Modelling and Simulation

In descending order of preference: (Alan Howling personal opinion!)

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

A. Howling Nankai University
March 28 - April 3 (2010)

1) ANALYTIC SOLUTION:

- gives physical understanding. Understand the ideal case before simulations.

- gives explicit scaling dependence of physical parameters.

- only applicable to simple cases, and simple cases often correspond to uniform situation. But if not uniform, then less interesting for applications!

- try to make each parameter separately uniform (e/m, composition, flow etc) for robust processing conditions and a wide operation window. Avoid empirical compensation of combinations of non-uniform parameters!

- useful to benchmark numerical simulation for confirmation and confidence (a numerical solution, if it converges, gives an answer. But is it correct?)

2) NUMERICAL CALCULATION OF ANALYTIC SOLUTION (eg Matlab programme)

3) NUMERICAL SOLUTION OF EQUATIONS (eg FlexPDE partial differential equation solver)

4) NUMERICAL SIMULATION (eg Siglo-RF; and COMSOL Multiphysics finite elements)

Industry prefers full 3D plasma + many chemical reactions in their CAD design. Good luck!

1) ANALYTIC SOLUTION EXAMPLES

• cylindrical reactor standing wave for parallel plates

• cylindrical reactor standing wave correction with lens electrode

• showerhead 1D gas flow

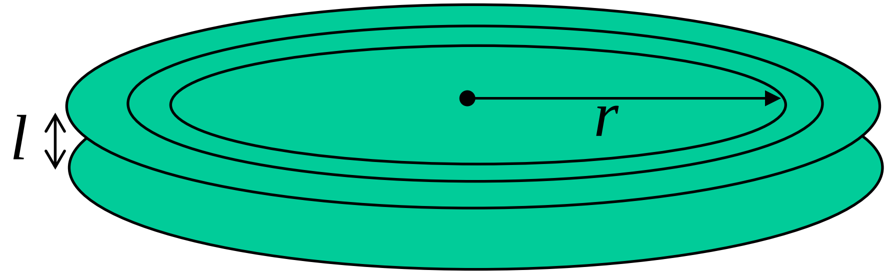
• 0D plasma chemistry, depletion and microcrystallinity.

• time-resolved, equilibration time, dispersive axial flow

• wavefield solutions

Admittance of cylindrical parallel plates, gap l

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE



Capacitance of parallel plates, $C = \dfrac{\varepsilon_0 A}{l}$

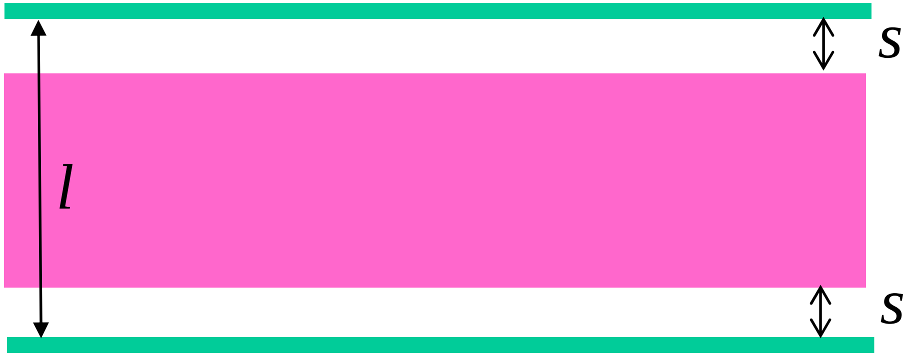
Elemental cylindrical capacitance, $dC = \dfrac{\varepsilon_0 2\pi r\, dr}{l}$

Capacitance per unit length in cylinder along r $= \dfrac{\varepsilon_0 2\pi r}{l}$

Capacitive impedance $= \dfrac{1}{\mathrm{j}\omega C}$, admittance $= \mathrm{j}\omega C$.

Admittance per unit length of cylindrical parallel plates, $Y = \mathrm{j}\omega \dfrac{\varepsilon_0 2\pi r}{l}$

Effective permittivity of plasma-&-sheaths



Plasma short-circuits the transverse electric field:

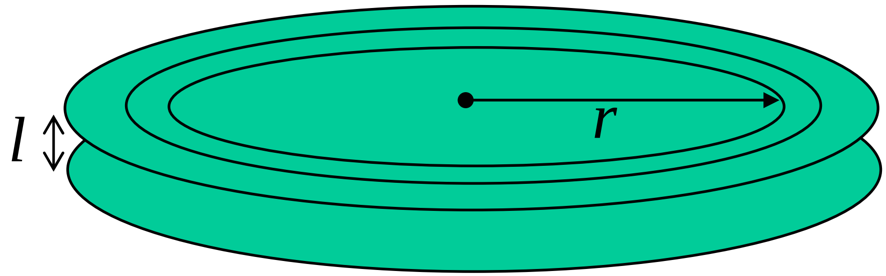
Combined capacitance of sheaths $= \dfrac{\varepsilon_0 A}{2s}$,

Effective capacitance of the gap $= \dfrac{\varepsilon_0 \varepsilon_{\text{eff}} A}{l}$,

$\therefore$ Effective permittivity of the gap, $\varepsilon_{\text{eff}} = \dfrac{l}{2s}$. ($\varepsilon_{\text{eff}} = 1$ sans plasma; since $2s = l$)

$$\boxed{\text{Effective admittance per unit length of plasma-\&-sheaths in cylindrical parallel plates, } Y = \mathrm{j}\omega\varepsilon_0\varepsilon_{\text{eff}}\frac{2\pi r}{l}.}$$

Series impedance of cylindrical parallel plates, gap l



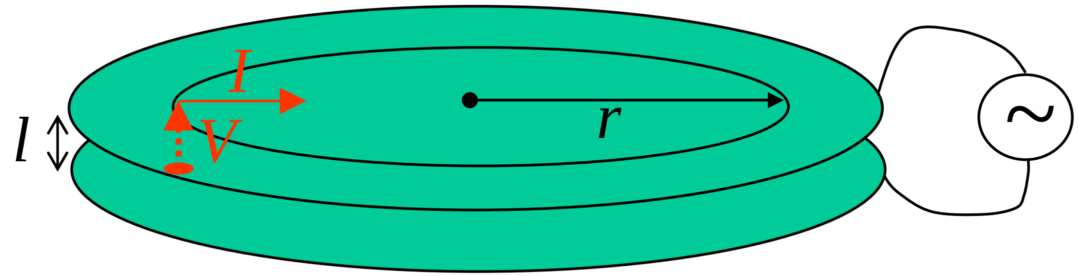
Inductance of cylindrical element, $dL = \dfrac{\mu_0 l \, dr}{2\pi r}$,

Impedance of cylindrical element $= \mathrm{j}\omega \dfrac{\mu_0 l \, dr}{2\pi r}$.

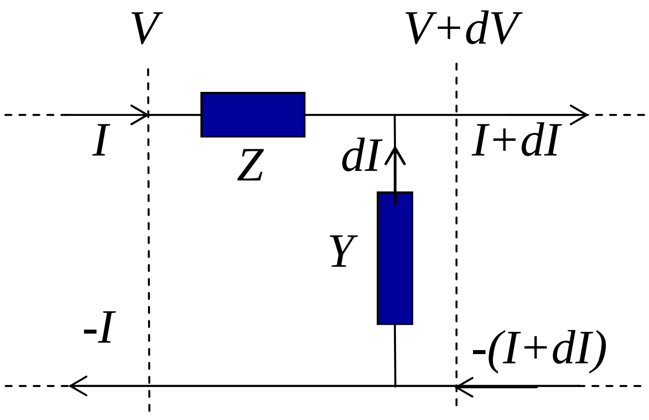
Series impedance in cylinder per unit length along r, is $Z = \mathrm{j}\omega\mu_0 \dfrac{l}{2\pi r}$.

Consider a *general* cylindrical transmission line

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE



Uniform voltage and current around the circumference, open circuit on axis, series impedance Z, and parallel admittance Y, per unit length along r.



Kirchoff's laws: $\dfrac{dV}{dr} = -IZ, \quad \dfrac{dI}{dr} = -YV.$

Substitute for I (or for V):

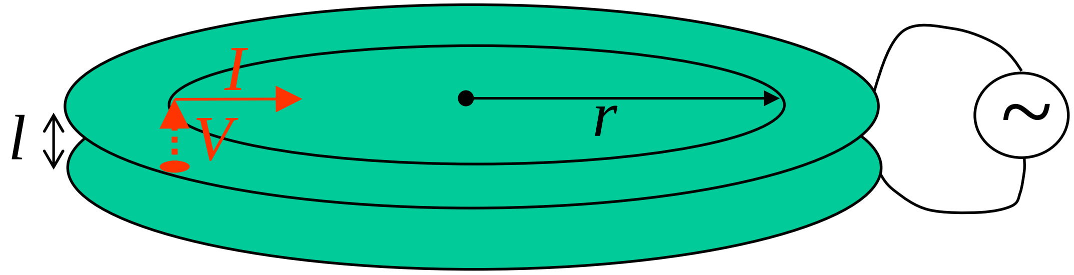
$$\boxed{\frac{d^2V}{dr^2} = \left(\frac{1}{Z}\frac{dZ}{dr}\right)\frac{dV}{dr} + YZV,}$$

which is the *general* voltage wave equation for a cylindrical transmission line.

Consider a *parallel-plate* cylindrical transmission line

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

l is constant,
V is variable.



Use the parallel-plate expressions: $Z = \mathrm{j}\omega\mu_0 \dfrac{l}{2\pi r}, \quad Y = \mathrm{j}\omega\varepsilon_0\varepsilon_{\text{eff}} \dfrac{2\pi r}{l}$

$\therefore \left(\dfrac{1}{Z}\dfrac{dZ}{dr}\right) = -\dfrac{1}{r}$ and the general cylindrical transmission line equation is:

$\boxed{\dfrac{d^2V}{dr^2} + \dfrac{1}{r}\dfrac{dV}{dr} + k^2V = 0,}$ which is the voltage wave equation which gives a zero-order Bessel function solution for parallel-plate cylindrical geometry,

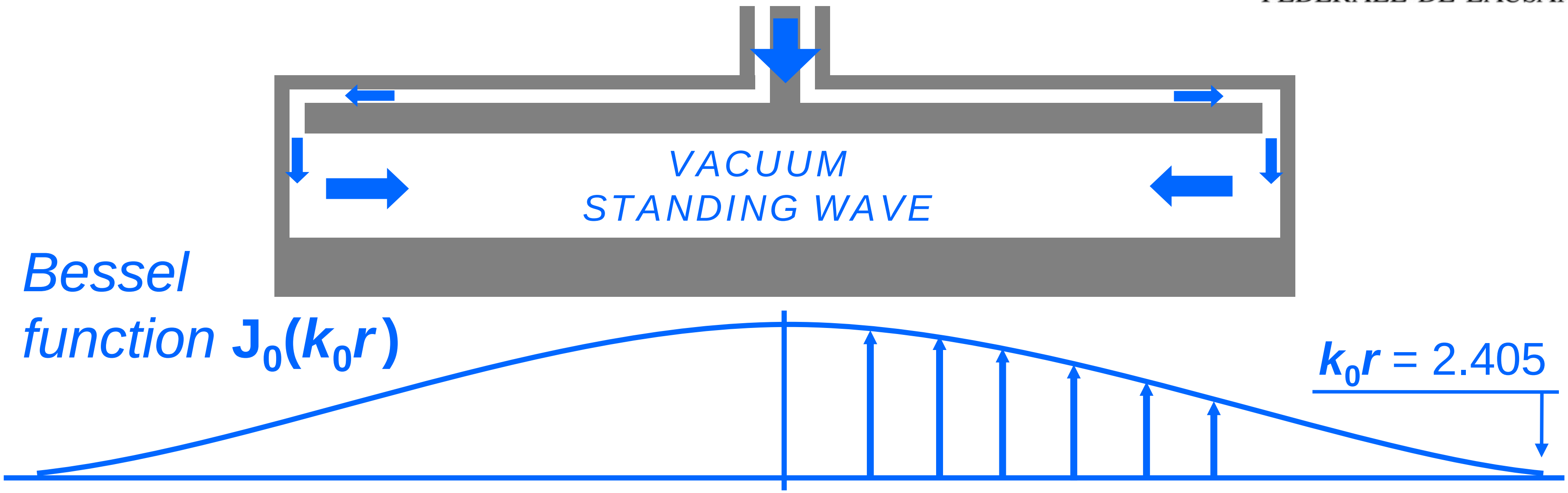
where $k^2 = -YZ = \omega^2\mu_0\varepsilon_0\varepsilon_{\text{eff}} = k_0^2\varepsilon_{\text{eff}}$;

i.e. $k = k_0\varepsilon_{\text{eff}}$, and the wave phase velocity $= \dfrac{1}{\sqrt{\mu_0\varepsilon_0\varepsilon_{\text{eff}}}} = \dfrac{c}{\sqrt{\varepsilon_{\text{eff}}}}$.

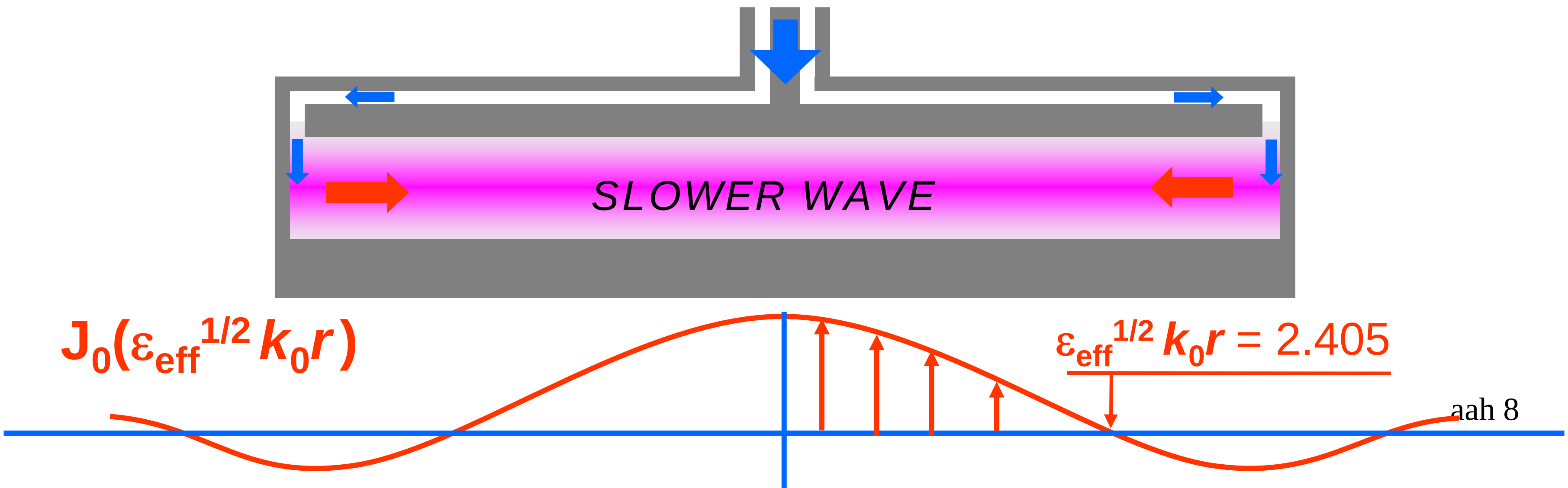
(sheath width s & ε_{eff} have been assumed independent of V)

Bessel function standing waves, parallel plates

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE



ε_{eff} "plasma equivalent dielectric" acts as a **worsening factor** for uniformity:



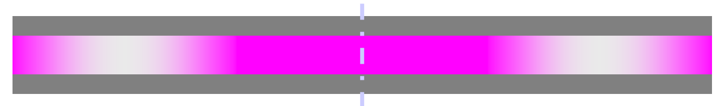
courtesy of Jacques Schmitt

Bessel function standing waves, parallel plates at 100 MHz

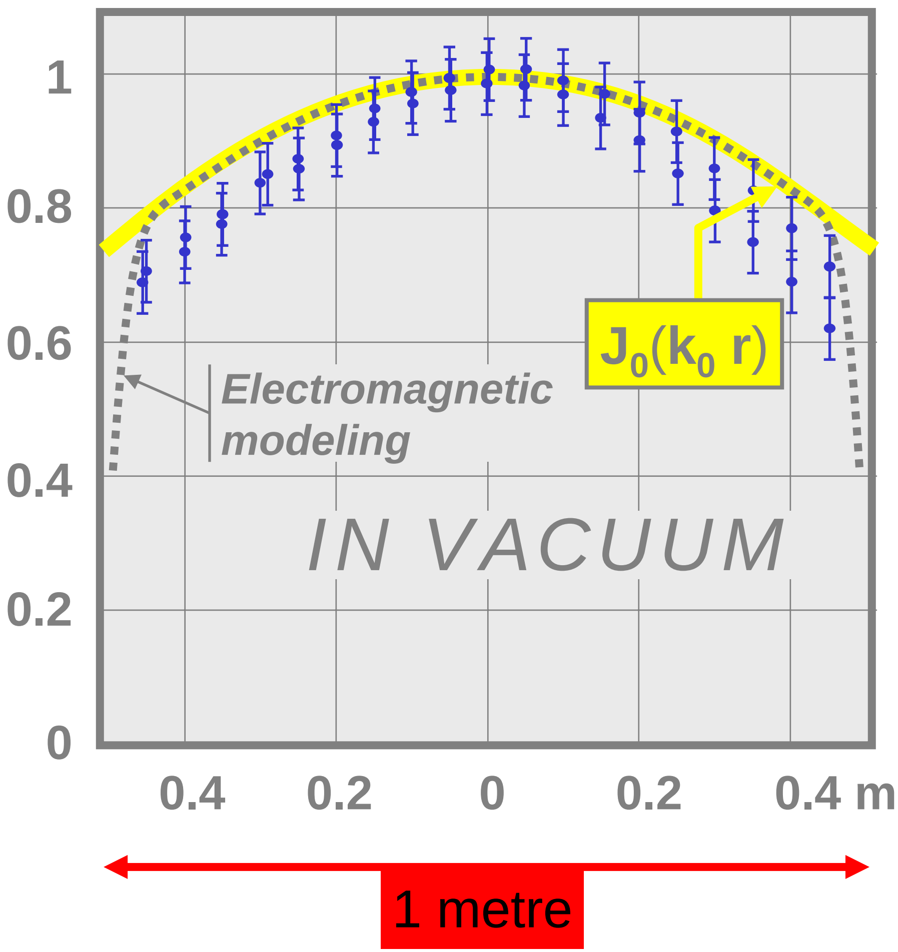
J. Appl. Phys. **95** 4559 (2004)

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

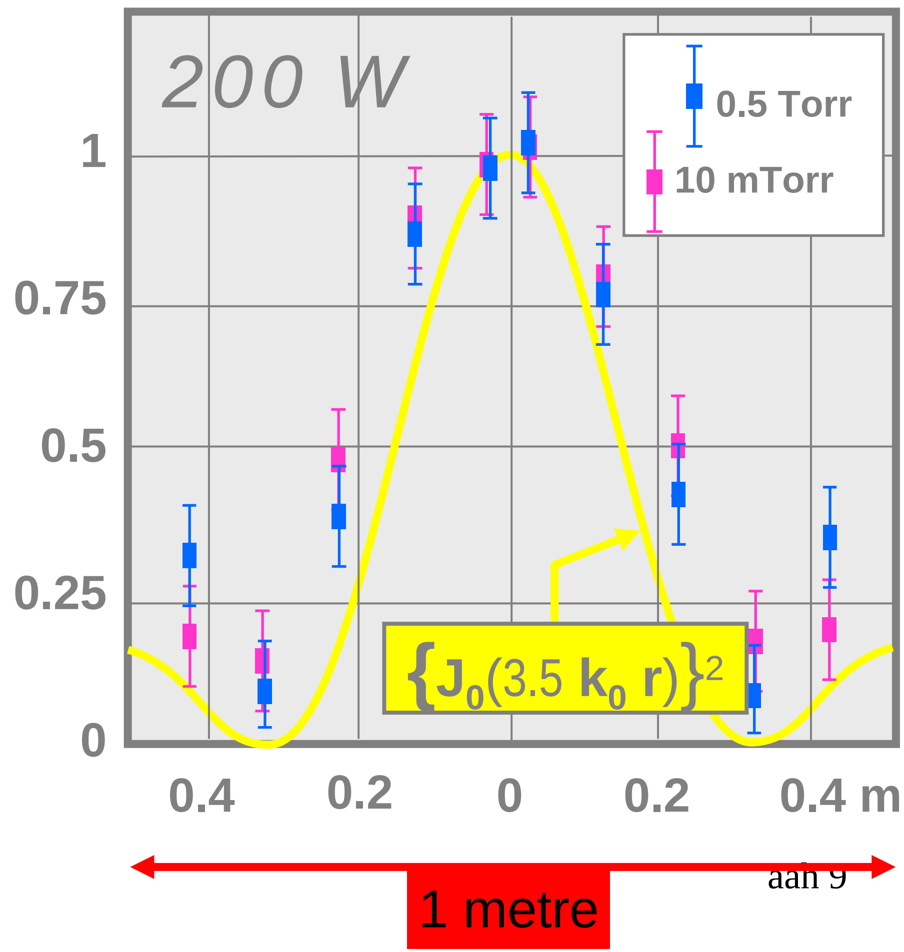
worsening factor with plasma means that the first node falls inside the reactor!



E-field



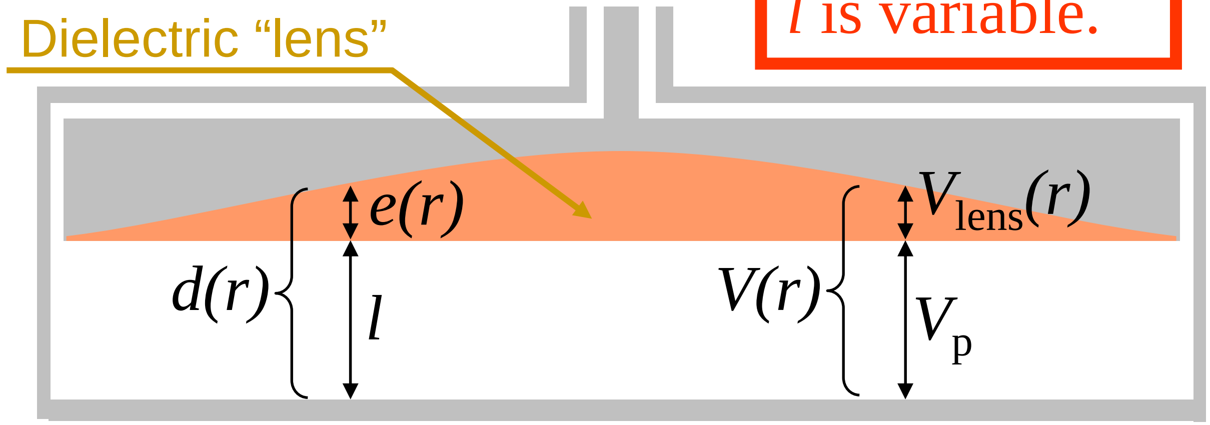
probe array ion saturation currents



World's Simplest Lens Solution

adapted from: P. Chabert *et al*, Phys. Pl. 11, 4081 (2004).

V_p is constant,
l is variable.



We keep a constant plasma gap, l,

but add a variable thickness lens $e(r)$.

Total electrode gap is now $d(r) = l + e(r)$.

The plasma voltage is V_p, which we *define* constant,

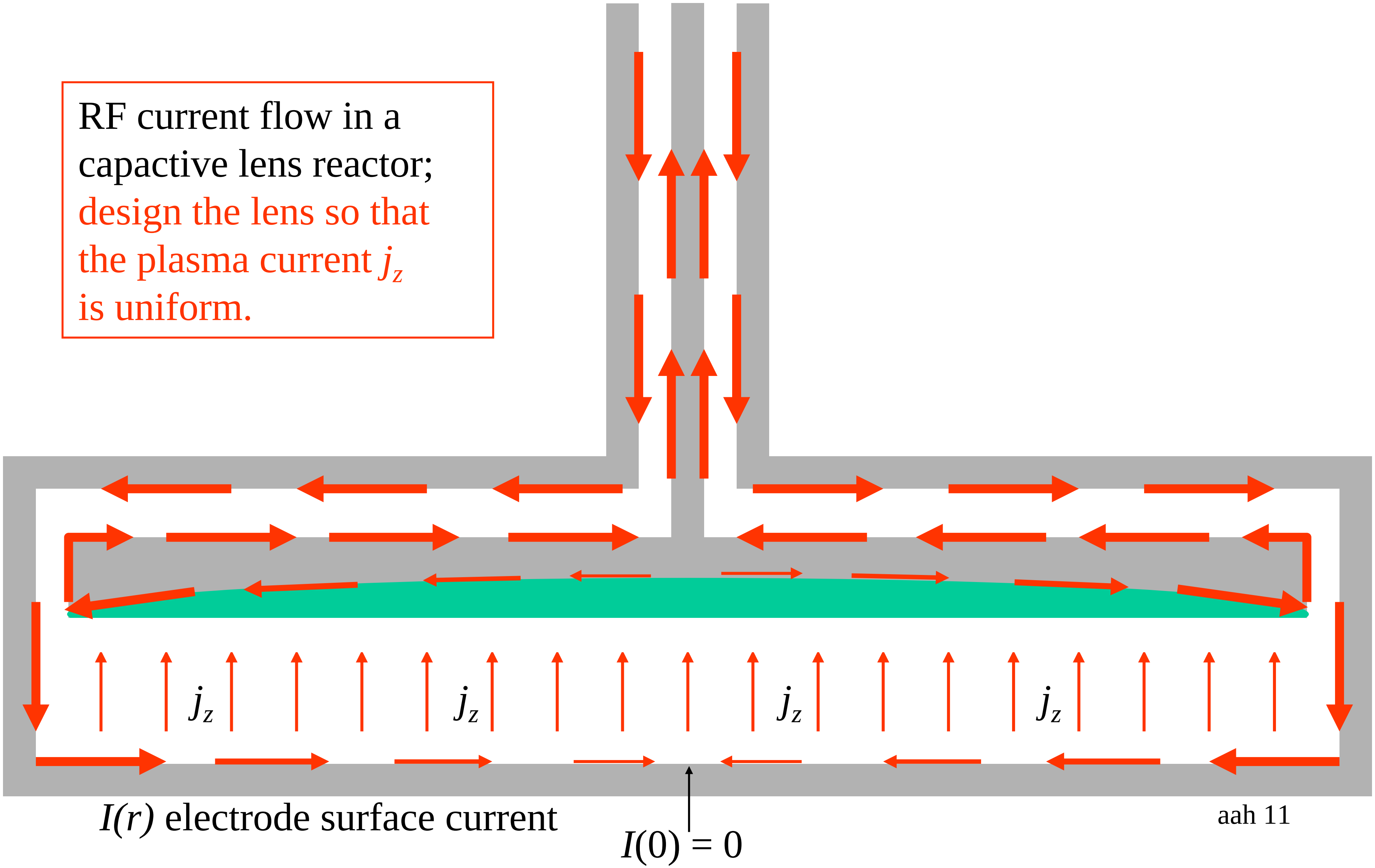
the voltage across the lens thickness is $V_{lens}(r)$.

The total electrode voltage is $V(r) = V_p + V_{lens}(r)$.

World's Simplest Lens Solution; introduction

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

RF current flow in a capactive lens reactor; design the lens so that the plasma current j_z is uniform.

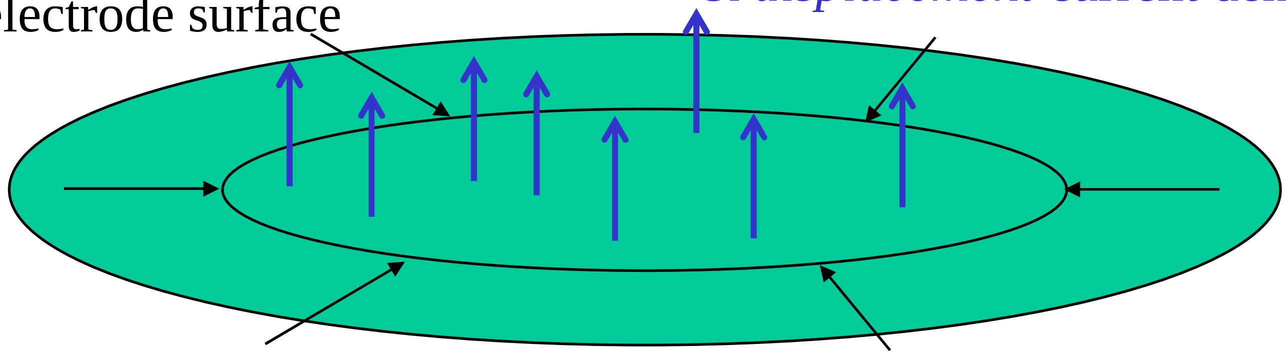


World's Simplest Lens Solution, I.

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

total radial *conduction* current =*I(r)* along the electrode surface

constant vertical electric field E_z & *displacement* current density, j_z



1) We require a constant vertical electric field in gap, $E_z = \dfrac{V_\mathrm{p}}{l} = \text{const.}$

2) $\therefore$ require constant vertical current density $j_z = \dfrac{\mathrm{j}\omega\varepsilon_0\varepsilon_\mathrm{eff}V_\mathrm{p}}{l} = \boxed{\dfrac{\mathrm{j}\omega\varepsilon_0\varepsilon_\mathrm{r}V_\mathrm{lens}(r)}{e(r)}}.$

3) The radial current in electrodes, $I(r) = -j_z\pi r^2$

(all the current entering radius r radially, must leave vertically,

because $I(0) = 0$, and j_z = constant over all r.)

World's Simplest Lens Solution, II.

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

4) To calculate $V(r)$, use Ohm's law radially: $dV(r) = -I(r)Z(r)dr$,

where $Z(r) = \mathrm{j}\omega\mu_0 \dfrac{d(r)}{2\pi r}$ is the series impedance of the gap, per unit radius.

5) Substitute: $\dfrac{dV(r)}{dr} = j_z \pi r^2 Z = \dfrac{\mathrm{j}\omega\varepsilon_0\varepsilon_\mathrm{r} V_\mathrm{lens}(r)}{e(r)} \pi r^2 \cdot \mathrm{j}\omega\mu_0 \dfrac{d(r)}{2\pi r}$,

$\therefore \quad \dfrac{dV_\mathrm{lens}(r)}{dr} = -k_0^2 \varepsilon_\mathrm{r} V_\mathrm{lens}(r) \dfrac{d(r)}{e(r)} \dfrac{r}{2}$, since $V(r) = V_\mathrm{lens}(r) + V_\mathrm{p}$.

6) Substitute for $V_\mathrm{lens}(r)$ using 2): $V_\mathrm{lens}(r) = \dfrac{\varepsilon_\mathrm{eff}}{\varepsilon_\mathrm{r}} \dfrac{V_\mathrm{p}}{l} e(r)$ so that

$e'(r) = -k_0^2 \varepsilon_\mathrm{r} d(r) \dfrac{r}{2}$, and since $d(r) = e(r) + l$, $d'(r) = -k_0^2 \varepsilon_\mathrm{r} d(r) \dfrac{r}{2}$.

7) $\boxed{\therefore \; d(r) = \left(l + e(0)\right) \exp\left(\dfrac{-k_0^2 \varepsilon_\mathrm{r} r^2}{4}\right), \text{ a Gaussian lens.}}$

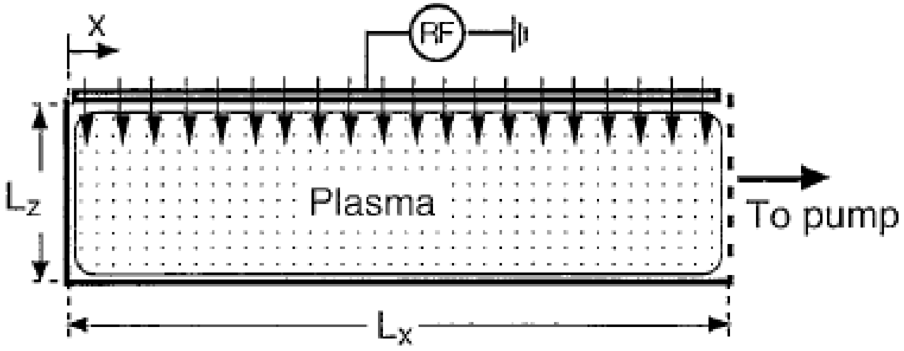
Lens shape depends on ε_r, not ε_eff. $\therefore$ Lens shape independent of plasma.

A gas flow uniformity study in large-area showerhead reactors for RF plasma deposition

L Sansonnens, A A Howling and Ch Hollenstein

Plasma Sources Sci. Technol. 9 (2000) 205–209.

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE



simple 1D model suggests that gas composition is spatially uniform across a showerhead reactor with a uniform plasma,

i.e. a 0D model can be justified for a large area showerhead reactor

basic plasma chemistry

plasma dissociation: $AB_2 + e \xrightarrow{k_d} AB + B + e$ (1)

surface reactions: $AB + \text{ surface } \xrightarrow{k_s} A_s + B$ (2)

species continuity equations

$$\frac{d}{dx}(n_{AB_2}v(x)) = D_{AB_2}\frac{d^2 n_{AB_2}}{dx^2} + \phi - k_d n_e n_{AB_2} \qquad (5)$$

$$\frac{d}{dx}(n_{AB}v(x)) = D_{AB}\frac{d^2 n_{AB}}{dx^2} + k_d n_e n_{AB_2} - k_s n_{AB} \qquad (6)$$

$$\frac{d}{dx}(n_B v(x)) = D_B\frac{d^2 n_B}{dx^2} + k_d n_e n_{AB_2} + k_s n_{AB} \qquad (7)$$

$$n_t = n_{AB_2} + n_{AB} + n_B = \text{ constant.}$$

unique solution

$$v(x) = a\,x \qquad \text{and} \qquad n_i = \text{ constant } \forall i$$

0-dimensional model; first order reaction rate balance for each species.

ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

flow in | lost by electron impact dissociation | inverse residence time (pumping loss)

$$\boxed{\mathrm{SiH_4}} \quad \Phi_{\mathrm{SiH_4}} - (kn_{\mathrm{e}} + a)n_{\mathrm{SiH_4}} = 0$$

produced by dissocation | lost by deposition

$$\boxed{\mathrm{SiH_2}} \quad kn_{\mathrm{e}}n_{\mathrm{SiH_4}} - Sn_{\mathrm{SiH_2}} = 0$$

flow in | produced by surface association | produced during deposition | lost by dissocation | inverse residence time (pumping loss)

$$\boxed{\mathrm{H_2}} \quad \Phi_{\mathrm{H_2}} + \frac{1}{2}Rn_{\mathrm{H}} + Sn_{\mathrm{SiH_2}} - (k_{\mathrm{H}}n_{\mathrm{e}} + a)n_{\mathrm{H_2}} = 0$$

$$\boxed{\mathrm{H}} \quad 2kn_{\mathrm{e}}n_{\mathrm{SiH_4}} + 2k_{\mathrm{H}}n_{\mathrm{e}}n_{\mathrm{H_2}} - Rn_{\mathrm{H}} = 0$$

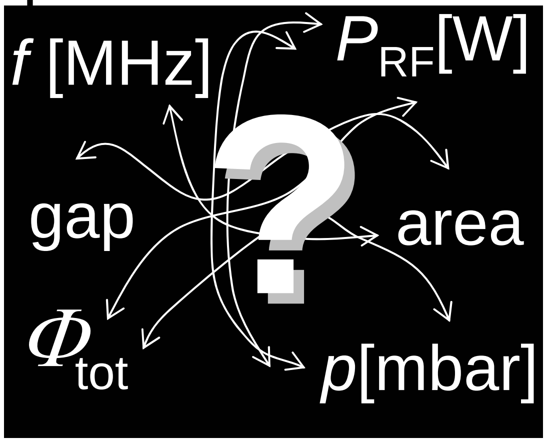
produced by dissocation of silane | produced by dissocation of hydrogen | loss rate by surface association

B. Strahm, A. A. Howling, L. Sansonnens and Ch. Hollenstein, *Plasma Sources Sci. Technol.* **16**, 80 (2007).

Depletion accounts for many of the plasma parameters

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

plasma black box



analytical model

$$\frac{k n_{\mathrm{e}}}{a_0} \doteq \left(\frac{1}{1-D}\right)\frac{D}{1+c(1-D)}$$

rate parameters in terms of concentration parameters

$a_0\left[\mathrm{s}^{-1}\right] =$ inverse residence time $=$ effective pumping speed $= 6.1 \cdot 10^{-6}\,\dfrac{T_{\mathrm{gas}}\Phi_{\mathrm{total}}}{p \cdot \mathrm{gap} \cdot \mathrm{area}}$;

$kn_{\mathrm{e}}\left[\mathrm{s}^{-1}\right] =$ silane dissociation rate $=$ plasma dissociation frequency $= F\left(P_{RF},\, f\,[\mathrm{MHz}]\right)$;

$c =$ silane input concentration, $\dfrac{\Phi_{\mathrm{SiH_4}}}{\Phi_{\mathrm{total}}}$.

Depletion scaling:

$$\boxed{D\uparrow \text{ if any of } \left\{p,\ \mathrm{gap},\ \mathrm{area},\ c,\ P_{\mathrm{RF}},\ f\right\}\uparrow \ \ \&/\text{or}\ \ \left\{F_{\mathrm{total}},\ T_{\mathrm{gas}}\right\}\downarrow}$$

B. Strahm, A. A. Howling, L. Sansonnens and Ch. Hollenstein, *Plasma Sources Sci. Technol.* **16**, 80 (2007).

Plasma chemistry equilibration 1/e time

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Plasma Sources Sci. Technol. **16** (2007) 679–696

Time-dependent 0-D analytical model :

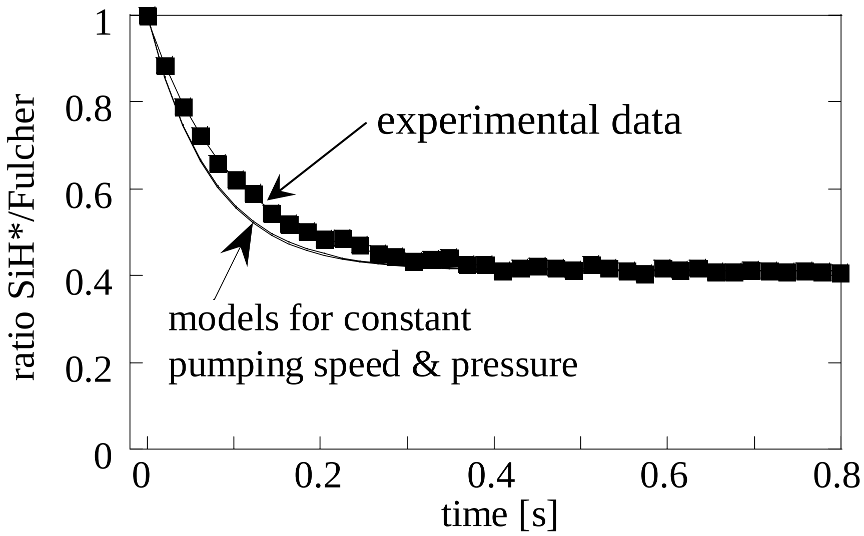
Assuming constant pumping speed, $a = a_0$,
the reaction rate balance for silane is

$$SiH_4 : \quad \Phi_{SiH_4} - (kn_e + a_0) n_{SiH_4} = \frac{dn_{SiH_4}}{dt}$$

$$\therefore \quad \frac{n_{SiH_4}(t)}{n_{SiH_4}(0)} = 1 - D\left[1 - \exp\left(-\frac{t}{\tau_{eq}}\right)\right],$$

where the plasma chemistry equilibration 1/e time, $\boxed{\tau_{eq} = \frac{(1-D)}{a_0} = \tau_{res}(1-D).}$

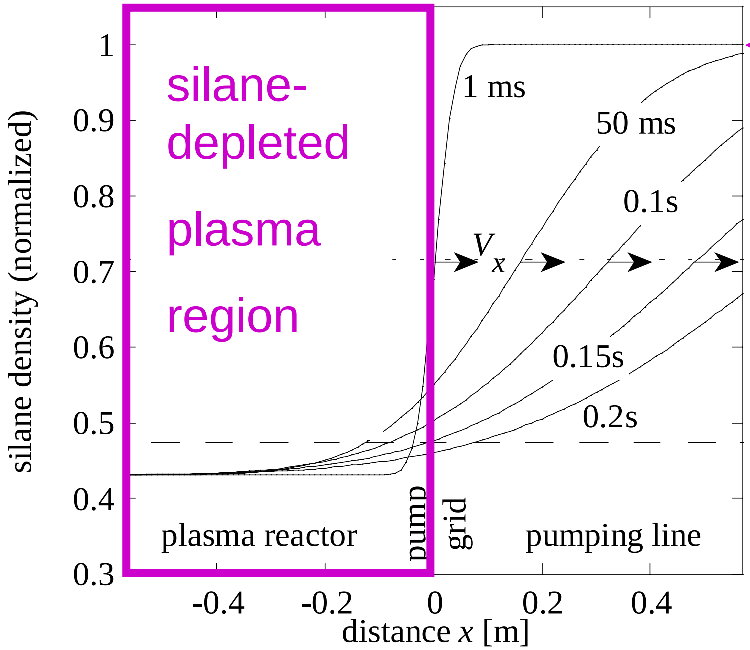
For this example, $\tau_{eq} = \frac{(1-0.57)}{5.7} = 0.076$ s.



good agreement with experiment

- the 0-D model was used to predict the required time resolution (~ 20 ms) of a spectrometer for experiments.

Dispersive axial flow from reactor along the pumping line



initial silane density in reactor and pumping line

Plasma Sources Sci. Technol. **16** (2007) 679–696

The general three-dimensional binary transfer equation for the vacuum chamber, equation (23), can now be simplified to a dispersive axial flow equation [9]:

$$\frac{\partial n_{\mathrm{SiH_4}}}{\partial t} + \bar{v}_x \frac{\partial n_{\mathrm{SiH_4}}}{\partial x} - D_{AB} \frac{\partial^2 n_{\mathrm{SiH_4}}}{\partial x^2} = 0, \qquad (24)$$

Analytic solution:

$$\frac{n_{\mathrm{SiH_4}}}{n^0_{\mathrm{SiH_4}}} = 1 - \frac{D}{2}\mathrm{erfc}(\zeta), \qquad \zeta = \frac{x - \bar{v}_x t}{(4 D_{AB} t)^{1/2}}$$

ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

2) NUMERICAL CALCULATION OF ANALYTIC SOLUTION (eg Matlab programme)

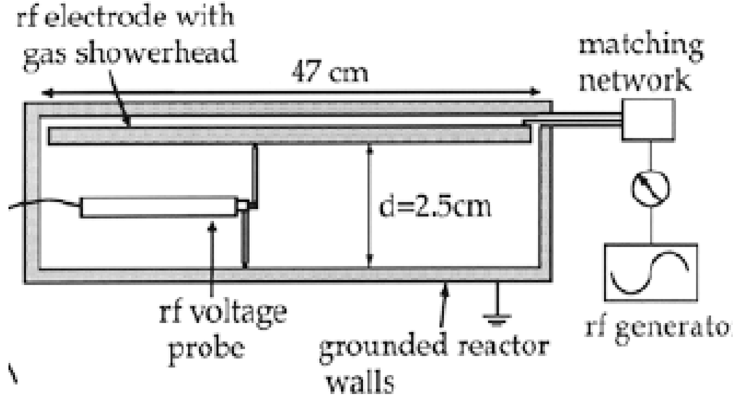
• Green's function solution for (vacuum) potential distribution, rectangular reactor

• wavefield graphs, cylindrical reactor

Voltage uniformity on parallel plates, using Green's functions (vacuum)

ECOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

L. Sansonnens *et al, Plasma Sources Sci. Technol.* **6**, 170 (1997)



Maxwell's equations reduce to a 2D driven Helmholtz equation (standing wave

$$(\nabla^2 + k^2)V(x) = i\omega\mu d J_z(x)$$

Green's function solution for a Dirac source:

$$(\nabla^2 + k^2)g(x; x_s) = \delta(x - x_s)$$

using eigenfunctions, defined

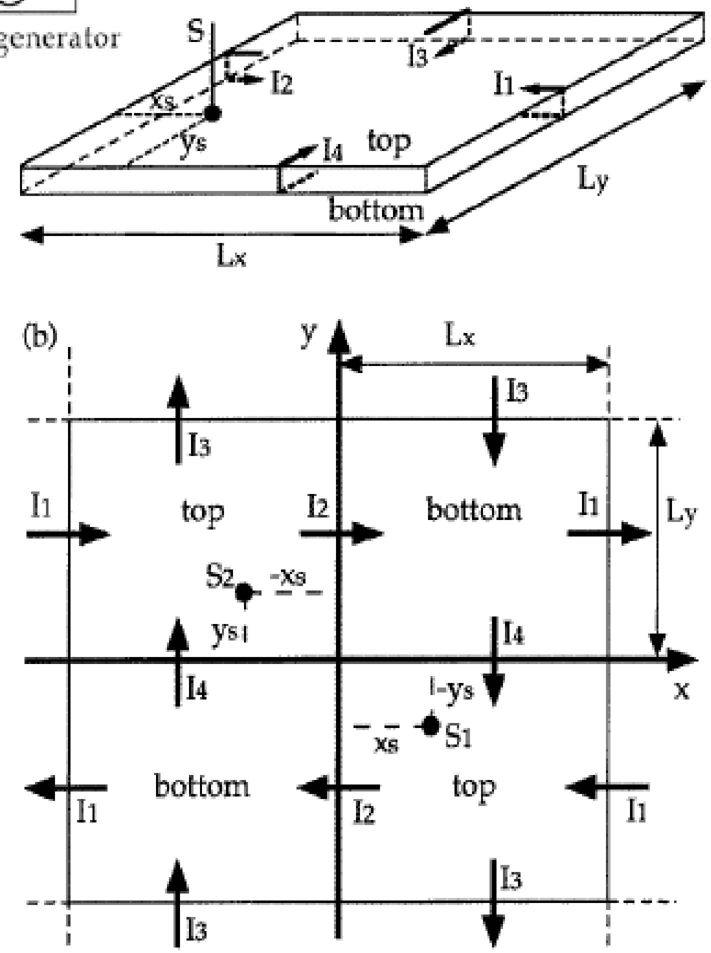
$$(\nabla^2 + k^2)\Phi_n(x) = \lambda_n \Phi_n(x)$$

express the Green's function

$$g(x; x_s) = \sum_n \frac{\Phi_n(x)\Phi_n(x_s)}{\lambda_n \langle \Phi_n, \Phi_n \rangle} \qquad \langle \Phi_n, \Phi_n \rangle \equiv \int d\Omega\, \Phi_n^2.$$

and the eigenfunctions are:

$$\Phi_n = \frac{\exp(i\pi(n_x x/L_x + n_y y/L_y))}{2\sqrt{L_x L_y}}$$

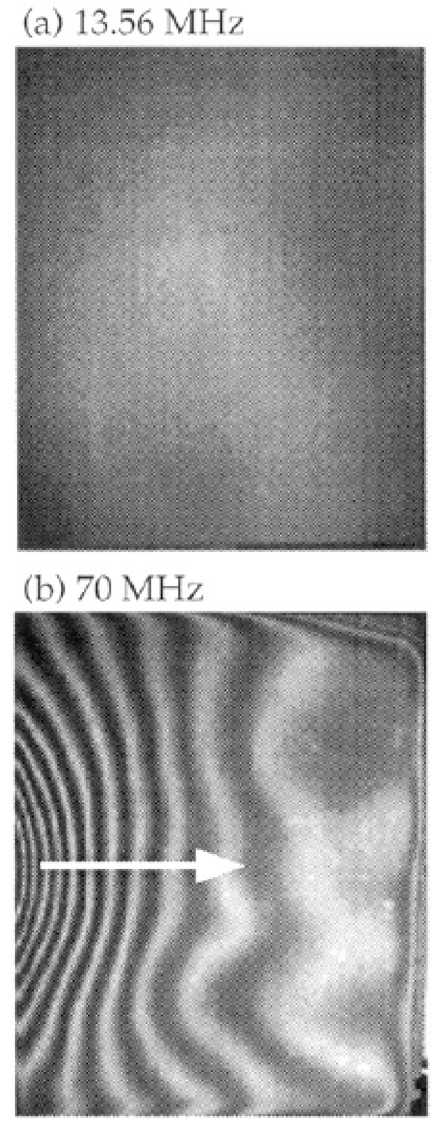


Voltage uniformity on parallel plates, using Green's functions (vacuum)

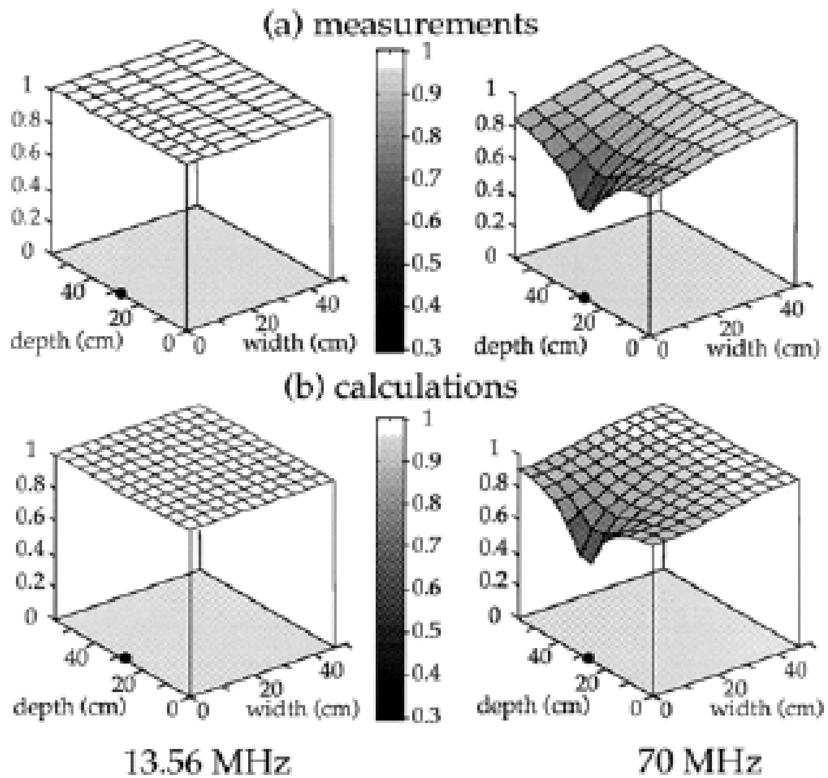
L. Sansonnens *et al, Plasma Sources Sci. Technol.* **6**, 170 (1997)

ECOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

thin film interferograms
(37 cm x 47 cm
substrate)



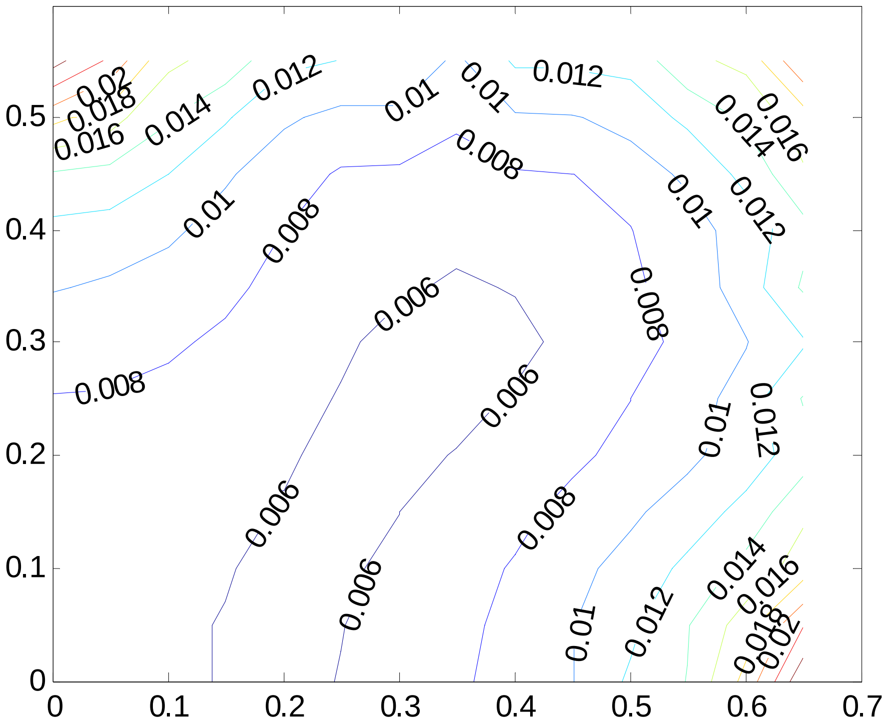
Green's function
model with
numerical
calculation
for voltage
distribution in
vacuum

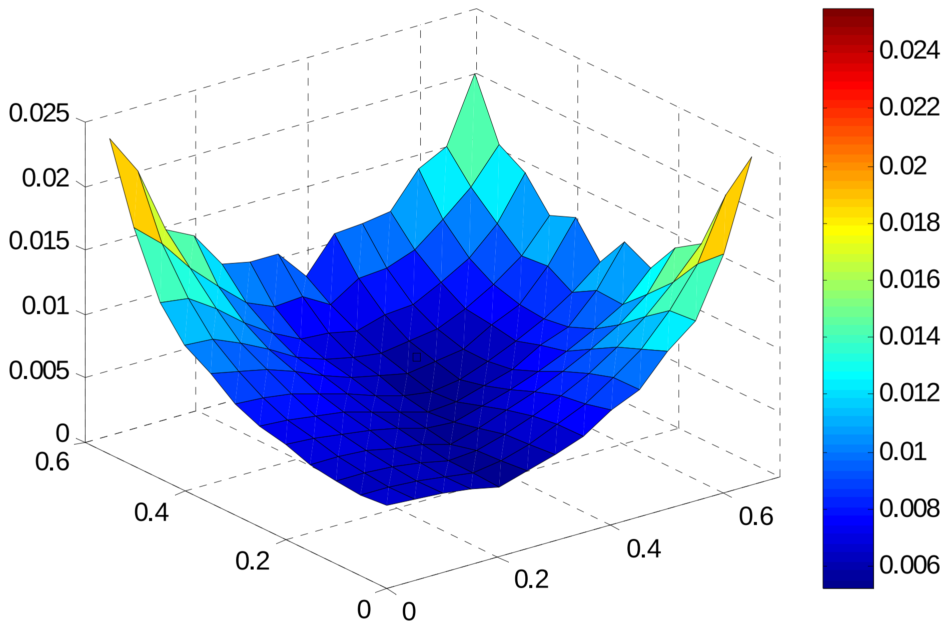


Estimate of best RF connection positions, using Green's functions (vacuum)

Define voltage non-uniformity $\Delta V = \dfrac{V_{\max} - V_{\min}}{V_{\max} + V_{\min}}$, electrode size 1.4 x 1.2 m, $f = 13.56$ MHz.

Plots of voltage non-uniformity vs RF connection position on a quadrant



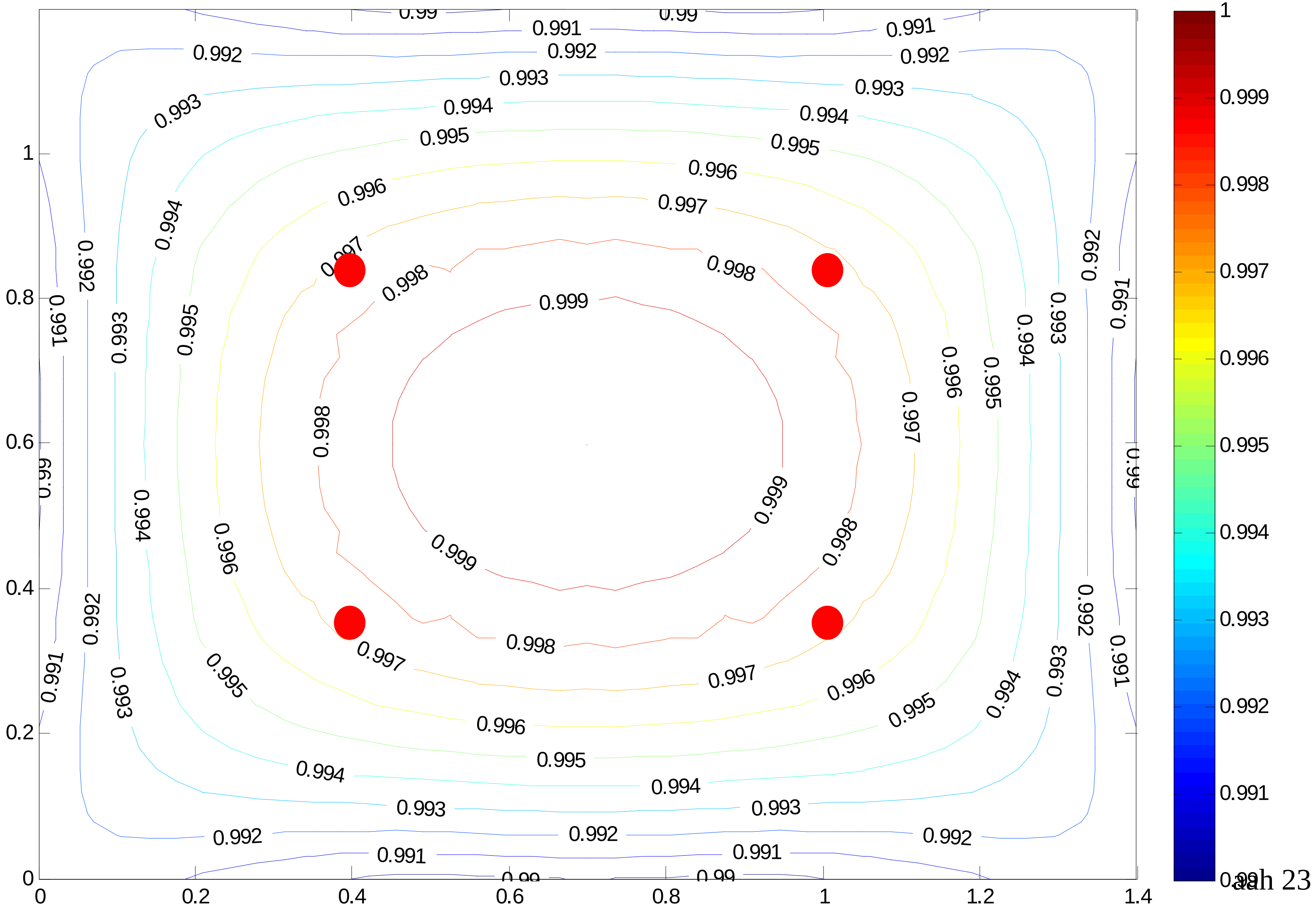


Position for best uniformity @ 13.56 MHz
4 connections: x ~ +/-0.3 m; y ~ +/-0.25 m;
ΔV ~ 0.0053

Estimate of best RF connection positions, using Green's functions (vacuum)

ÉCOLE POLYTECHNIQUE
USANNE

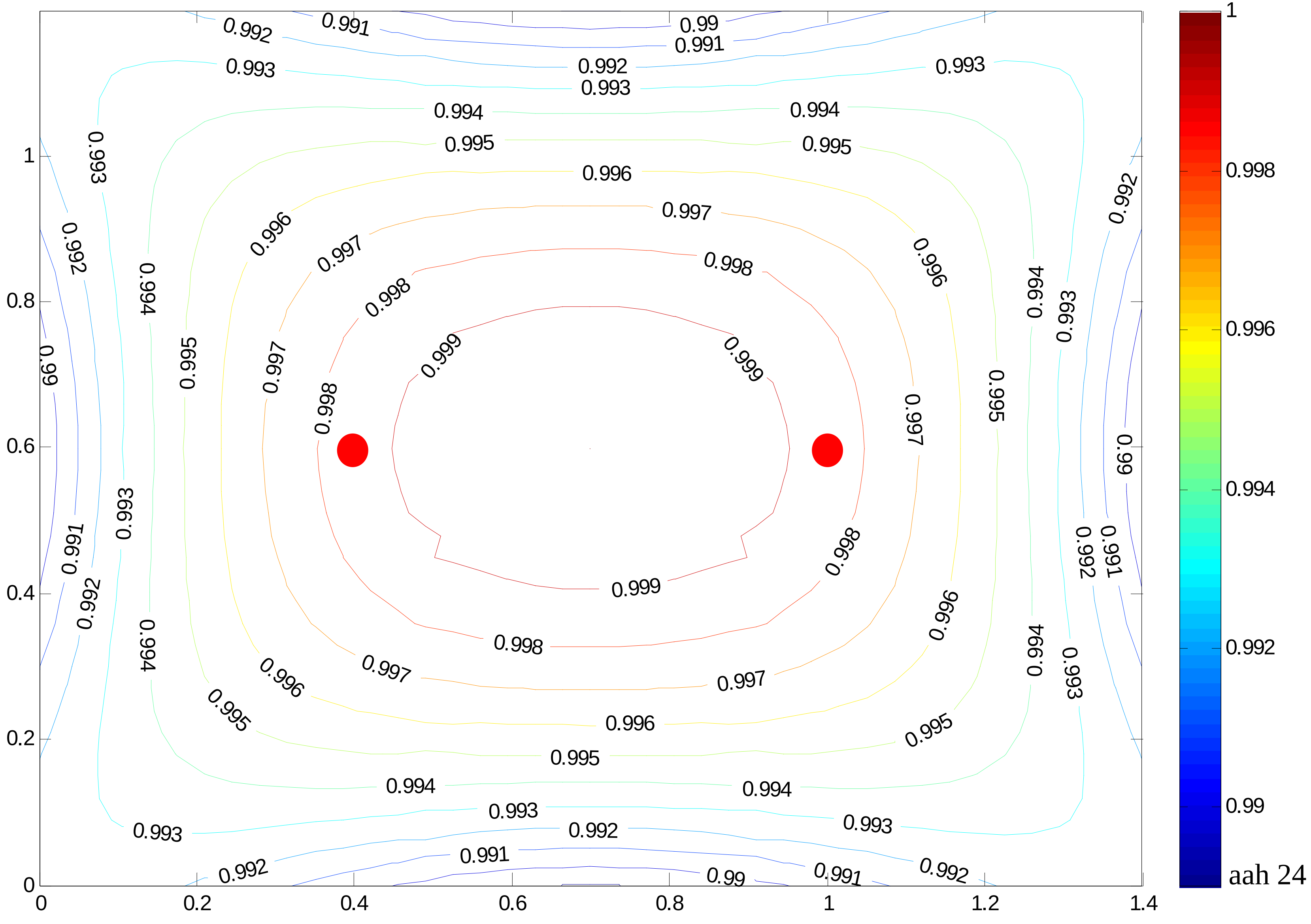
Voltage contour plot for 4 sources in best positions: x= +/-0.31 m, y= +/-0.24 m; 13.56 MHz



Estimate of best RF connection positions, using Green's functions (vacuum)

ECOLE POLYTECHNIQUE DE LAUSANNE

Voltage contour plot for 2 sources in best positions: x= +/-0.2 m, y= 0 m; 13.56 MHz



Wavefield equations in a cylindrical reactor with plasma

Plasma Sources Sci. Technol. 15 (2006) 302–313

Maxwell's equations

$$\frac{\partial H_\phi}{\partial z} = -\mathrm{j}\omega\epsilon_0\epsilon E_r,$$

$$\frac{1}{r}\frac{\partial(rH_\phi)}{\partial r} = \mathrm{j}\omega\epsilon_0\epsilon E_z,$$

$$\frac{\partial E_r}{\partial z} - \frac{\partial E_z}{\partial r} = -\mathrm{j}\omega\mu_0 H_\phi$$

field equation

$$\frac{1}{\epsilon}\left[\frac{\partial^2 H_\phi}{\partial r^2} + \frac{1}{r}\frac{\partial H_\phi}{\partial r} - \frac{1}{r^2}H_\phi\right] + \frac{\partial}{\partial z}\left[\frac{1}{\epsilon}\frac{\partial H_\phi}{\partial z}\right] + k_0^2 H_\phi = 0$$

general field solution for top sheath (here), plasma and bottom sheath regions

$$H_\phi = \sum_{n=0}^{\infty}\frac{D_n^{\mathrm{e}}}{K_{zs,n}^{\mathrm{e}}}\cos(K_{zs,n}^{\mathrm{e}}(l-z))J_1(K_{r,n}^{\mathrm{e}}r) + \sum_{n=0}^{\infty}\frac{D_n^{\mathrm{o}}}{K_{zs,n}^{\mathrm{o}}}\cos(K_{zs,n}^{\mathrm{o}}(l-z))J_1(K_{r,n}^{\mathrm{o}}r),$$

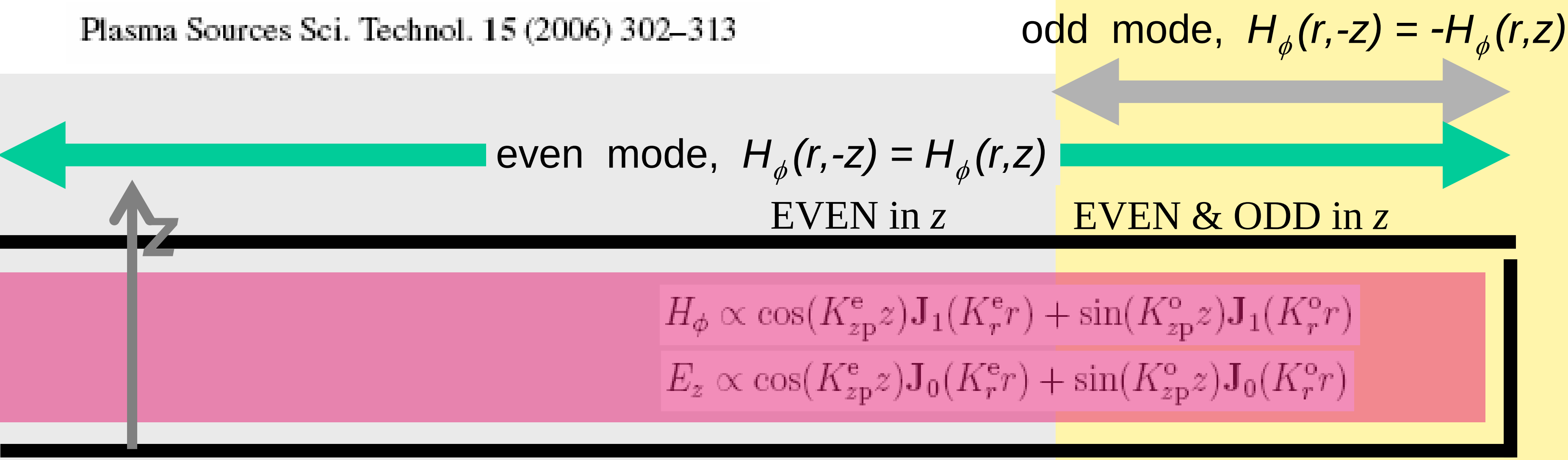
$$E_z = \frac{1}{\mathrm{j}\omega\epsilon_0}\sum_{n=0}^{\infty}\frac{D_n^{\mathrm{e}}K_{r,n}^{\mathrm{e}}}{K_{zs,n}^{\mathrm{e}}}\cos(K_{zs,n}^{\mathrm{e}}(l-z))J_0(K_{r,n}^{\mathrm{e}}r) + \frac{1}{\mathrm{j}\omega\epsilon_0}\sum_{n=0}^{\infty}\frac{D_n^{\mathrm{o}}K_{r,n}^{\mathrm{o}}}{K_{zs,n}^{\mathrm{o}}}\cos(K_{zs,n}^{\mathrm{o}}(l-z))J_0(K_{r,n}^{\mathrm{o}}r)$$

$$E_r = \frac{-1}{\mathrm{j}\omega\epsilon_0}\sum_{n=0}^{\infty}D_n^{\mathrm{e}}\sin(K_{zs,n}^{\mathrm{e}}(l-z))J_1(K_{r,n}^{\mathrm{e}}r) - \frac{1}{\mathrm{j}\omega\epsilon_0}\sum_{n=0}^{\infty}D_n^{\mathrm{o}}\sin(K_{zs,n}^{\mathrm{o}}(l-z))J_1(K_{r,n}^{\mathrm{o}}r).$$

find even and odd modes for symmetric and non-symmetric reactor, PTO

Wavefield equations in a cylindrical reactor with plasma

Plasma Sources Sci. Technol. 15 (2006) 302–313



the dispersion relation of the even mode reproduces the intuitive equivalent circuit of the standing wave effect:

$$(K^{\rm e}_{r,0})^2 \approx k_0^2 \frac{(1+d/s)}{(1+d/(\epsilon_{\rm p} s))}$$

$$= -{\rm j}\omega L_{\rm gap}\left[\frac{2}{{\rm j}\omega C_{\rm s}} + \frac{1}{Y_{\rm p}}\right]^{-1}$$

the dispersion relation of the odd mode reproduces the intuitive equivalent circuit of the telegraph effect:

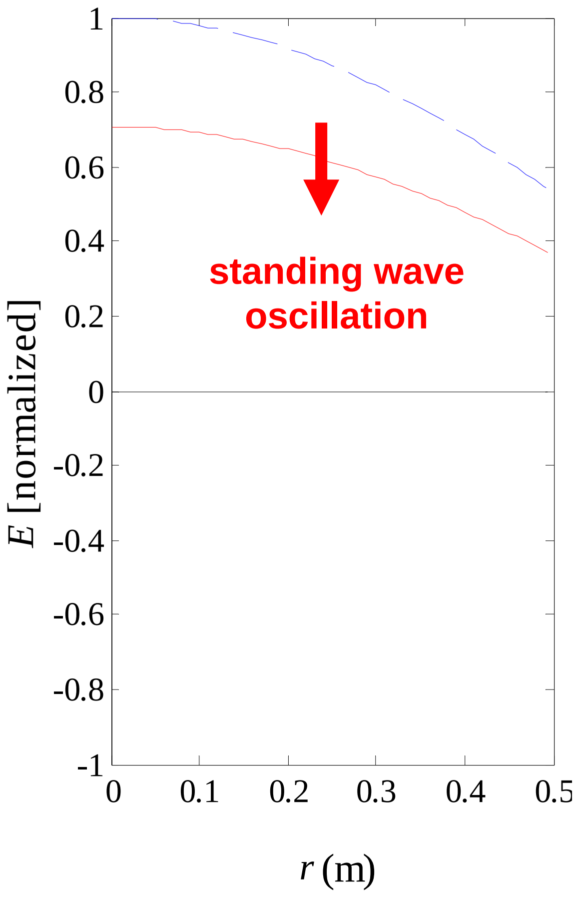
$$(K^{\rm o}_{r,0})^2 \approx k_0^2 - \frac{1}{\epsilon_{\rm p} s d}$$

$$= -\left[{\rm j}\omega L_{\rm s} + Z_{\rm sq}\right](2{\rm j}\omega C_{\rm s})$$

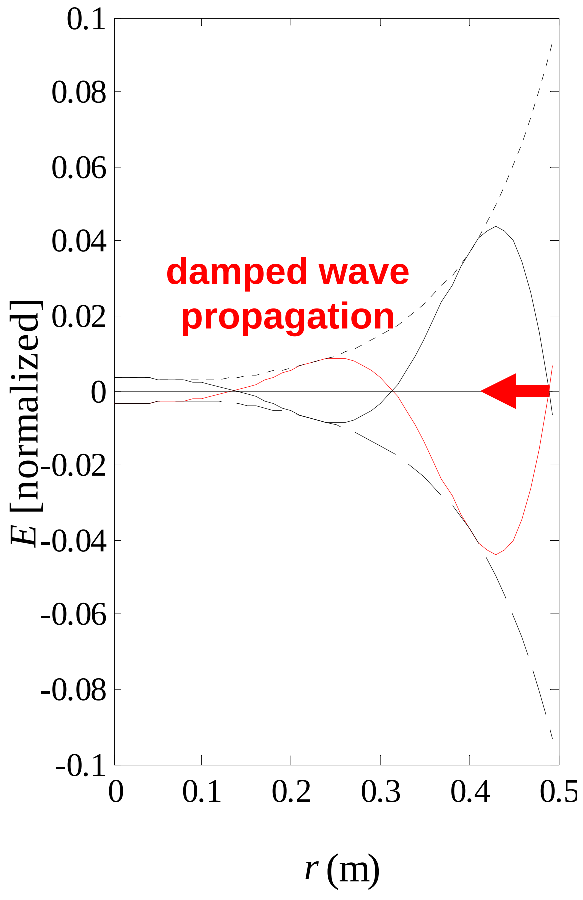
Wavefield analytic solution in a cylindrical reactor with plasma, solution plotted using Matlab

Plasma Sources Sci. Technol. 15 (2006) 302–313

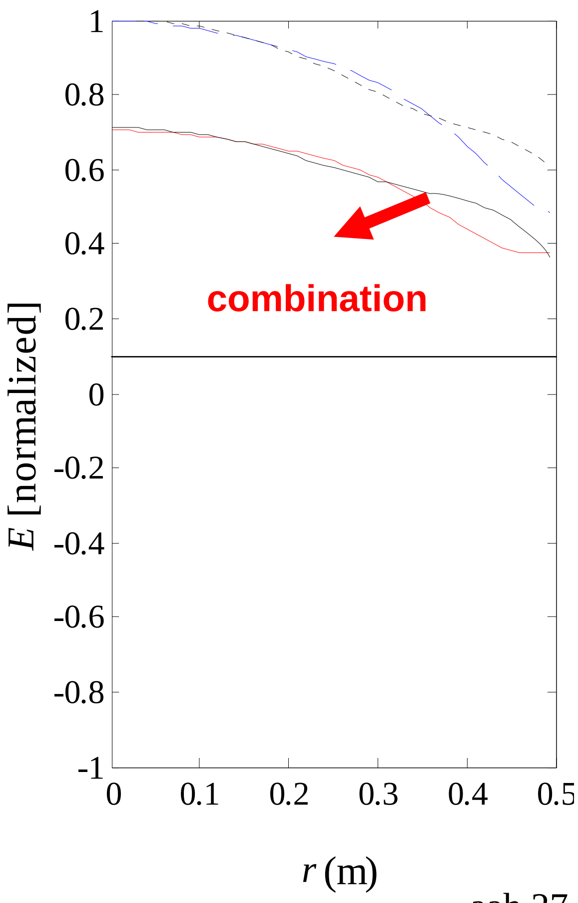
EVEN MODE
standing wave effect



ODD MODE
telegraph effect x10



PLASMA RESPONSE
combined effect



ÉCOLE POLYTECHNIQUE
FÉDÉRALE DE LAUSANNE

3) NUMERICAL SOLUTION OF EQUATIONS (eg FlexPDE partial differential equation solver)

• rectangular lens standing wave correction

• 2D rectangular telegraph effect

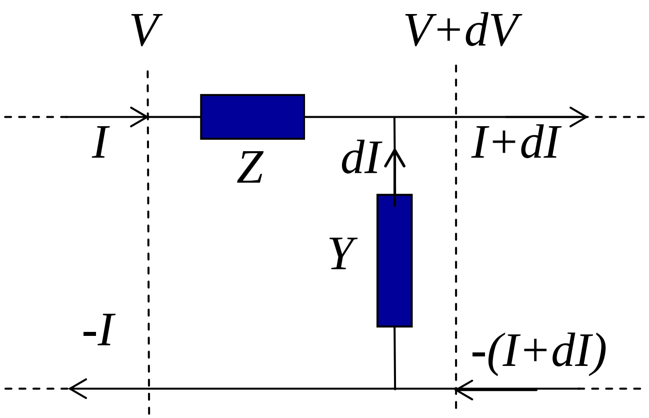
• plasma 2D benchmark in Comsol

Rectangular lens and standing wave correction

JOURNAL OF APPLIED PHYSICS 97, 063304 (2005)

L. Sansonnens

Reminder of cylindrical electrodes



Kirchoff's laws: $\frac{dV}{dr} = -IZ, \quad \frac{dI}{dr} = -YV.$

Substitute for I (or for V):

$\frac{d^2V}{dr^2} = \left(\frac{1}{Z}\frac{dZ}{dr}\right)\frac{dV}{dr} + YZV,$ which is the general voltage wave equation for a cylindrical transmission line.

Repeat for rectangular electrodes

Kirchoff's laws: $\nabla_t V = -Z\mathbf{J}_s, \quad \nabla_t \cdot \mathbf{J}_s = -YV + J_z$

Substitute for J (or for V):

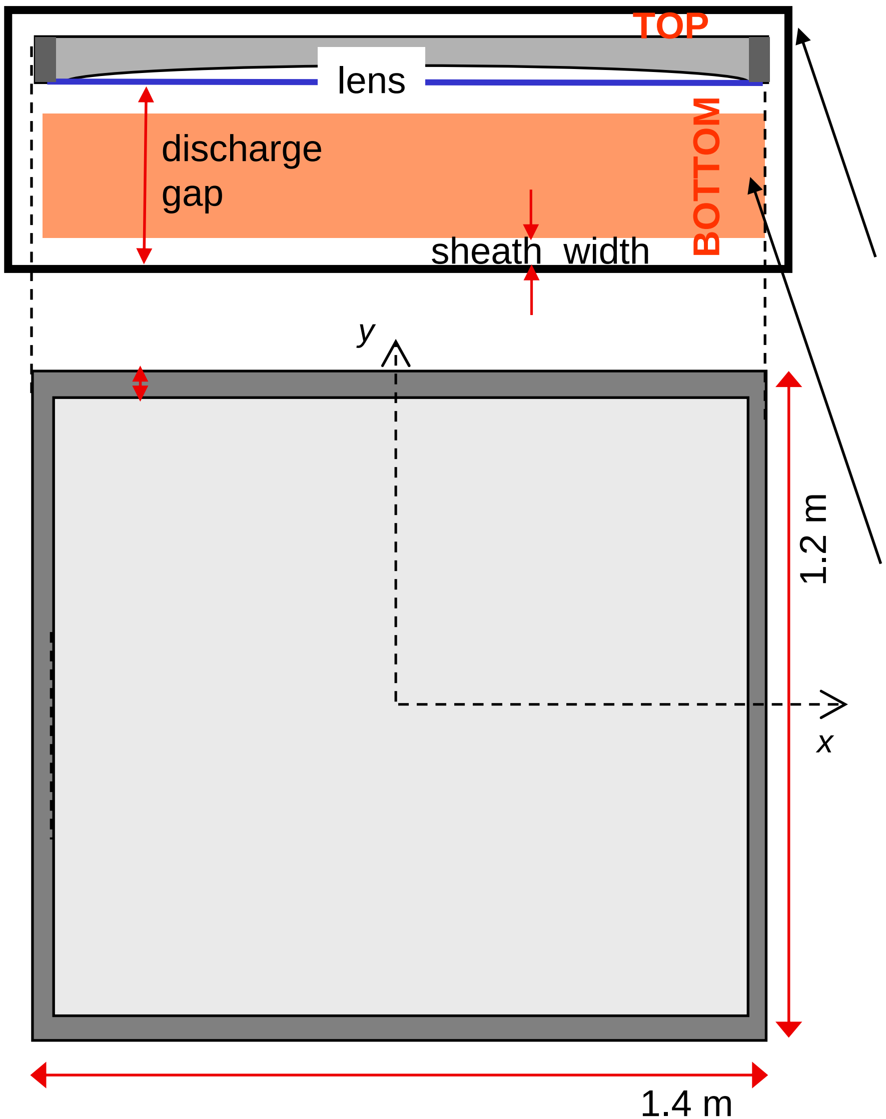
$$\nabla_t^2 V - \frac{\nabla_t Z}{Z} \cdot \nabla_t V - YZV = -ZJ_z.$$

which is the general voltage wave equation for a 2D quasiplanar circuit

Rectangular lens and standing wave correction

JOURNAL OF APPLIED PHYSICS 97, 063304 (2005) L. Sansonnens

1425 J. Vac. Sci. Technol. A 24(4), Jul/Aug 2006



Solve two wave equations:

for the voltage across the top, $V_{\text{top}}(x,y)$

and the voltage across the bottom, $V_{\text{bot}}(x,y)$.

Wave equation for the top gap (planar):

$$\nabla^2 V_{\text{top}} + k_0^2 V_{\text{top}} = f(x,y),$$

where $k_0^2 = \omega^2 / c^2$, f is the voltage source.

Wave equation for the bottom gap (curved):

$$\nabla^2 V_{\text{bot}} - \frac{\nabla d(x,y)}{d(x,y)} \cdot \nabla V_{\text{bot}} + k_{\text{eff}}^2 V_{\text{bot}} = 0,$$

where $k_{\text{eff}}^2 = \omega^2 \varepsilon_{\text{eff}}(x,y) / c^2$,

$\varepsilon_{\text{eff}}(x,y)$ accounts for the plasma, sheath and lens,

$d(x,y)$ accounts for the changing gap inductance

per unit area, $Z(x,y) = j\mu_0 \omega d(x,y)$.

Rectangular lens and standing wave correction

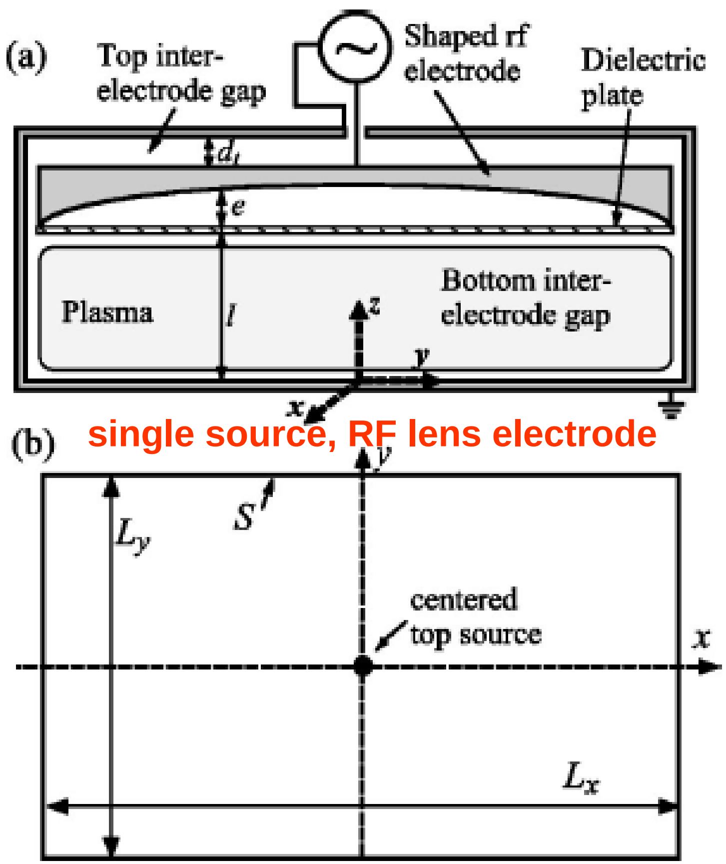
JOURNAL OF APPLIED PHYSICS 97, 063304 (2005)

L. Sansonnens 1425 J. Vac. Sci. Technol. A 24(4), Jul/Aug 2006

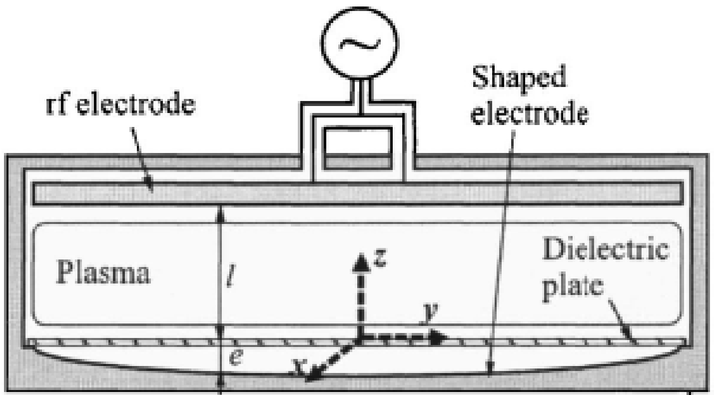
...along with the boundary conditions for voltage and surface current continuity:

$$V_{\text{top}} = V_{\text{bot}} \quad \text{and} \quad \frac{1}{Z_{\text{top}}}\frac{\partial V_{\text{top}}}{\partial \underline{n}} = \frac{1}{Z_{\text{bot}}}\frac{\partial V_{\text{bot}}}{\partial \underline{n}}.$$

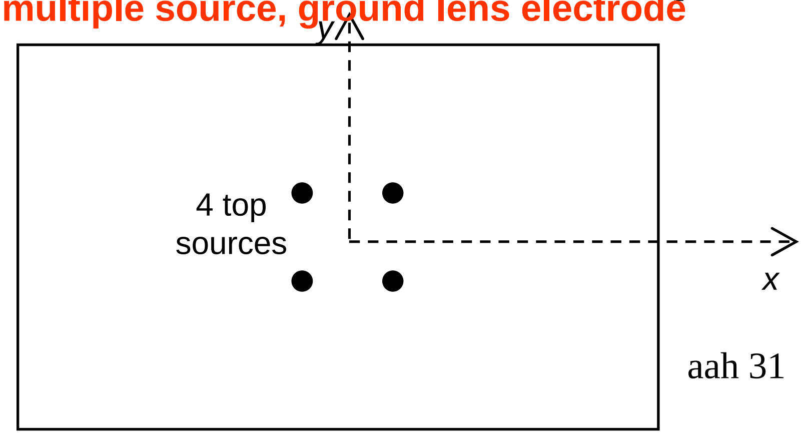
For RECTANGULAR electrodes, the boundary conditions, and therefore the lens shape, depend on the PLASMA.



single source, RF lens electrode



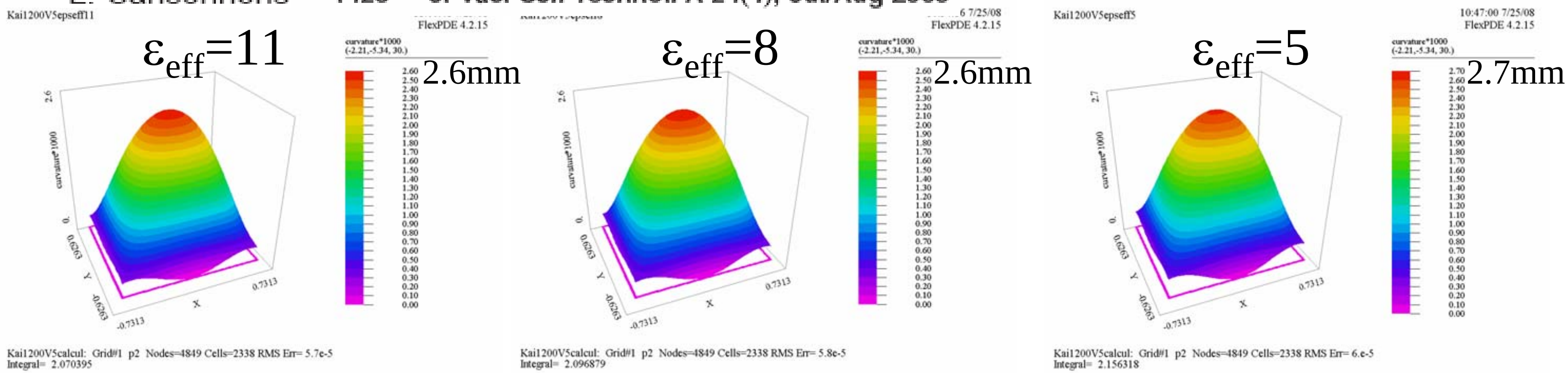
multiple source, ground lens electrode



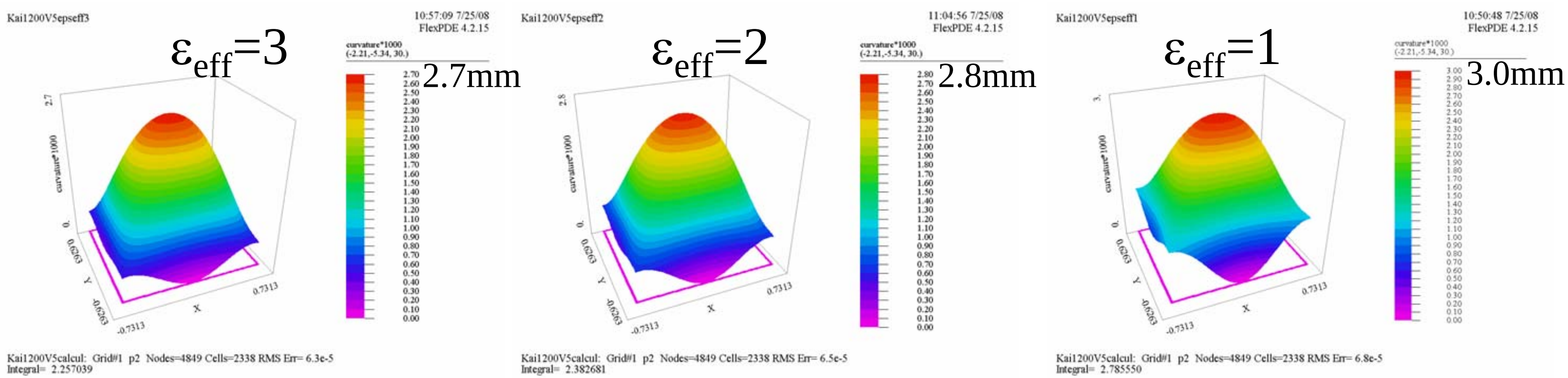
Rectangular lens shape: standing wave correction

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

L. Sansonnens 1425 J. Vac. Sci. Technol. A 24(4), Jul/Aug 2006



Laurent Sansonnens programme using FlexPDE solver. Luckily, the lens shape is not very sensitive to plasma.

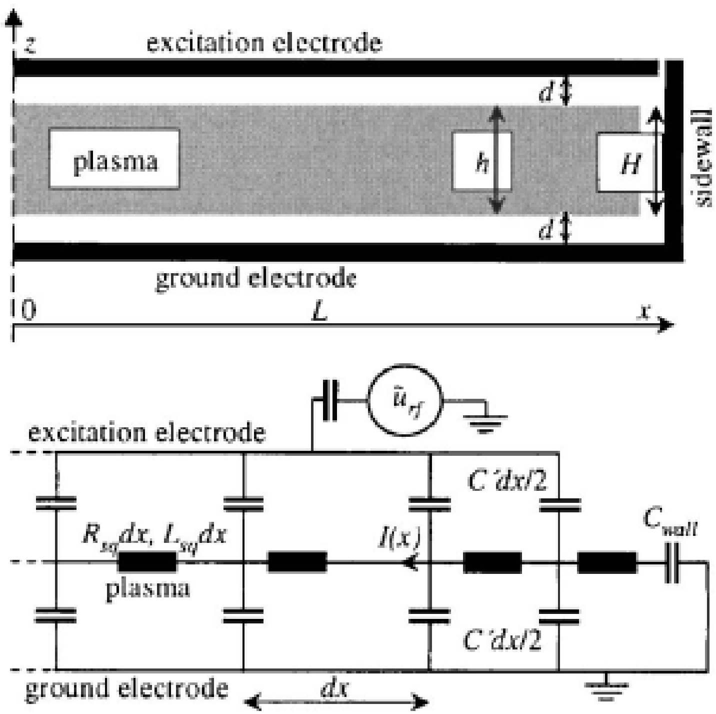


The boundary conditions depend on the top gap and sheaths.
Only for *cylindrical* lens is the shape independent of plasma.

2D calculation of the telegraph effect in rectangular reactors

JOURNAL OF APPLIED PHYSICS 97, 123308 (2005)
and J. Appl. Phys. **96**, 5429 (2004)

Injection of RF current from a sidewall along the plasma.



Equivalent circuit of the plasma and sheaths gives the 2D telegraph equation:

$$\nabla^2 V - L_{sq} C' \frac{\partial^2 V}{\partial t^2} - R_{sq} C' \frac{\partial V}{\partial t} = 0$$

The 1D analytic solution is:

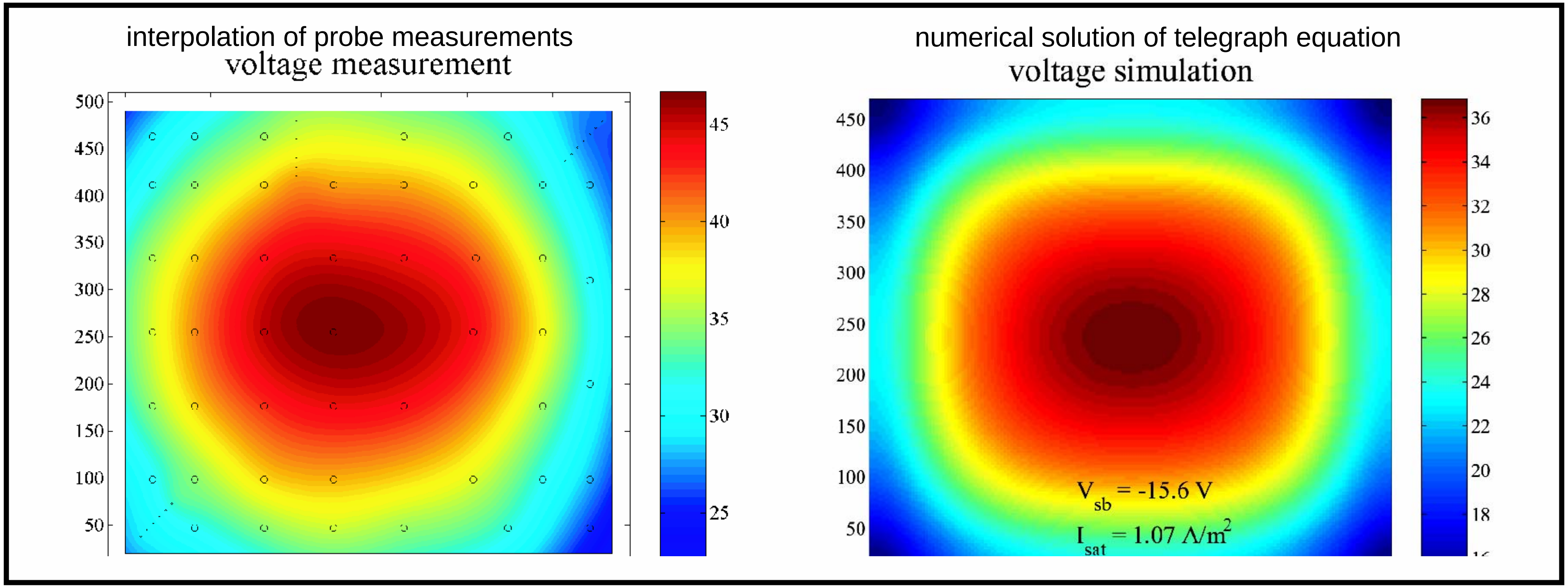
$$V = V_1 e^{-x/\delta} e^{i(\omega t - x/\delta)}$$

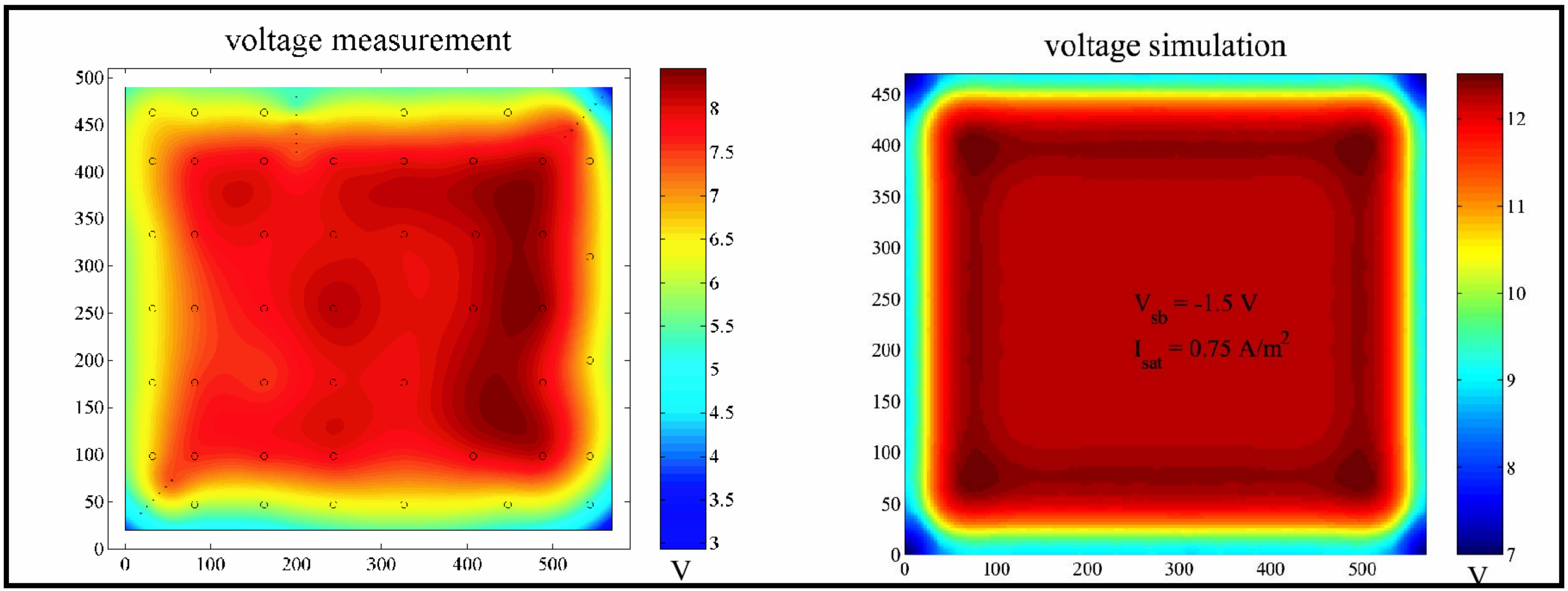
with damping length:

$$\delta = \sqrt{\frac{2}{\omega R_{sq} C'}} = \omega_{pe} \sqrt{\frac{hd}{\omega \nu_m}},$$

The equation to be solved numerically is

$$\nabla^2 \tilde{\mathbf{v}} = \frac{2}{\delta^2}\left(i - \frac{\omega}{\nu_m}\right)\tilde{\mathbf{v}},$$ **for 2D**

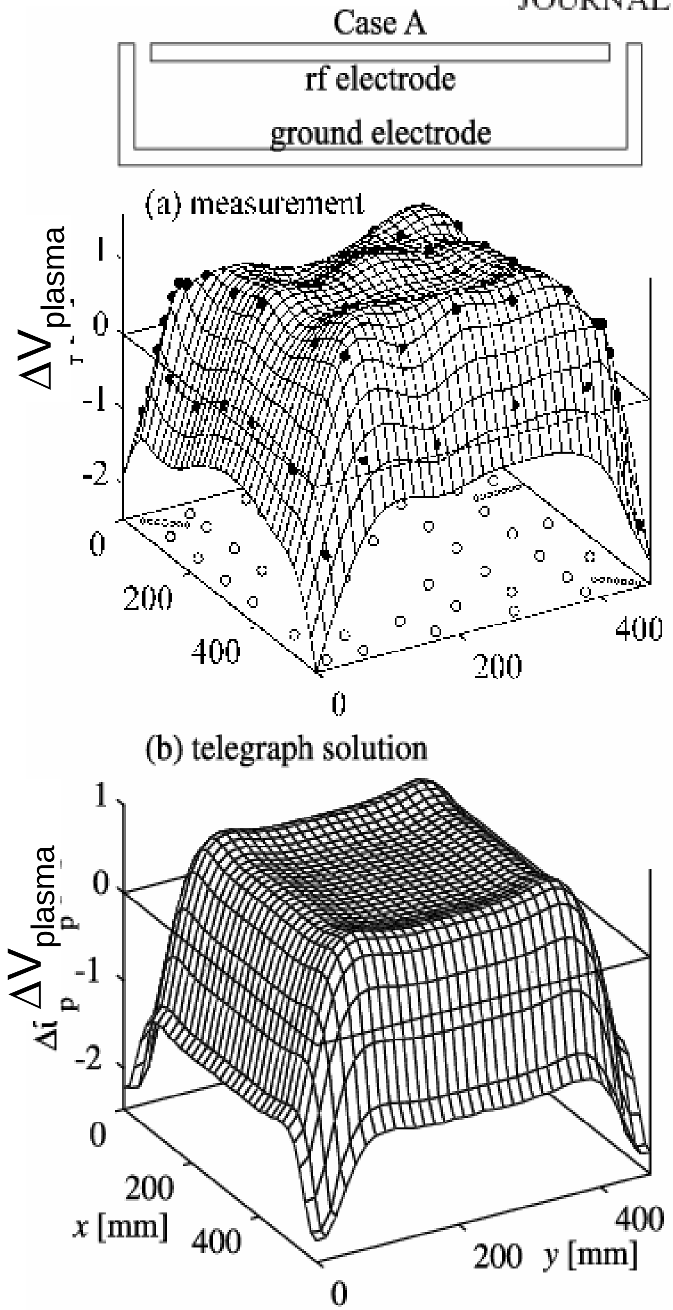

interpolation of probe measurements
voltage measurement
numerical solution of telegraph equation
voltage simulation
V sb = -15.6 V
I sat = 1.07 A/m2


voltage measurement
V
voltage simulation
V sb = -1.5 V
I sat = 0.75 A/m2
V

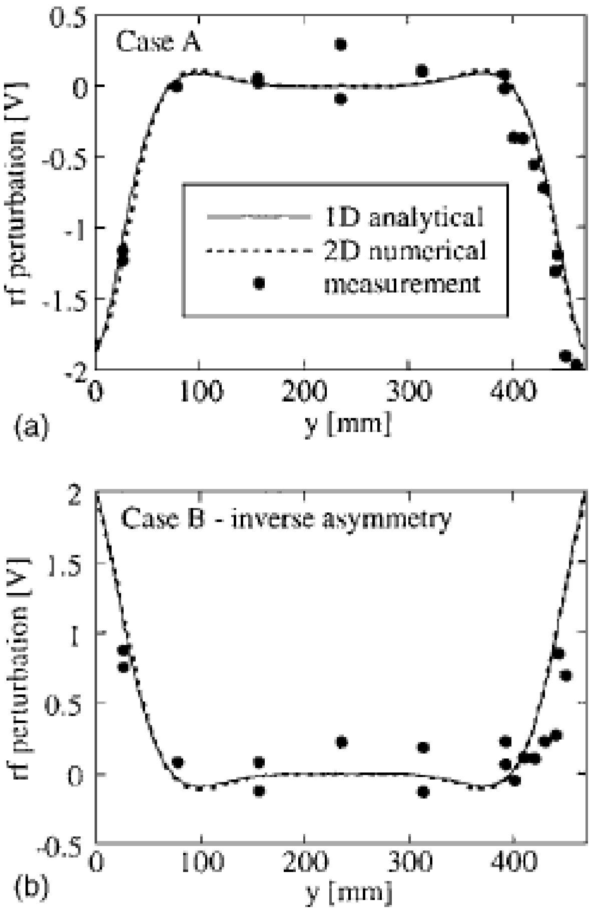
2D calculation of the telegraph effect in rectangular reactors

JOURNAL OF APPLIED PHYSICS 97, 123308 (2005)

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

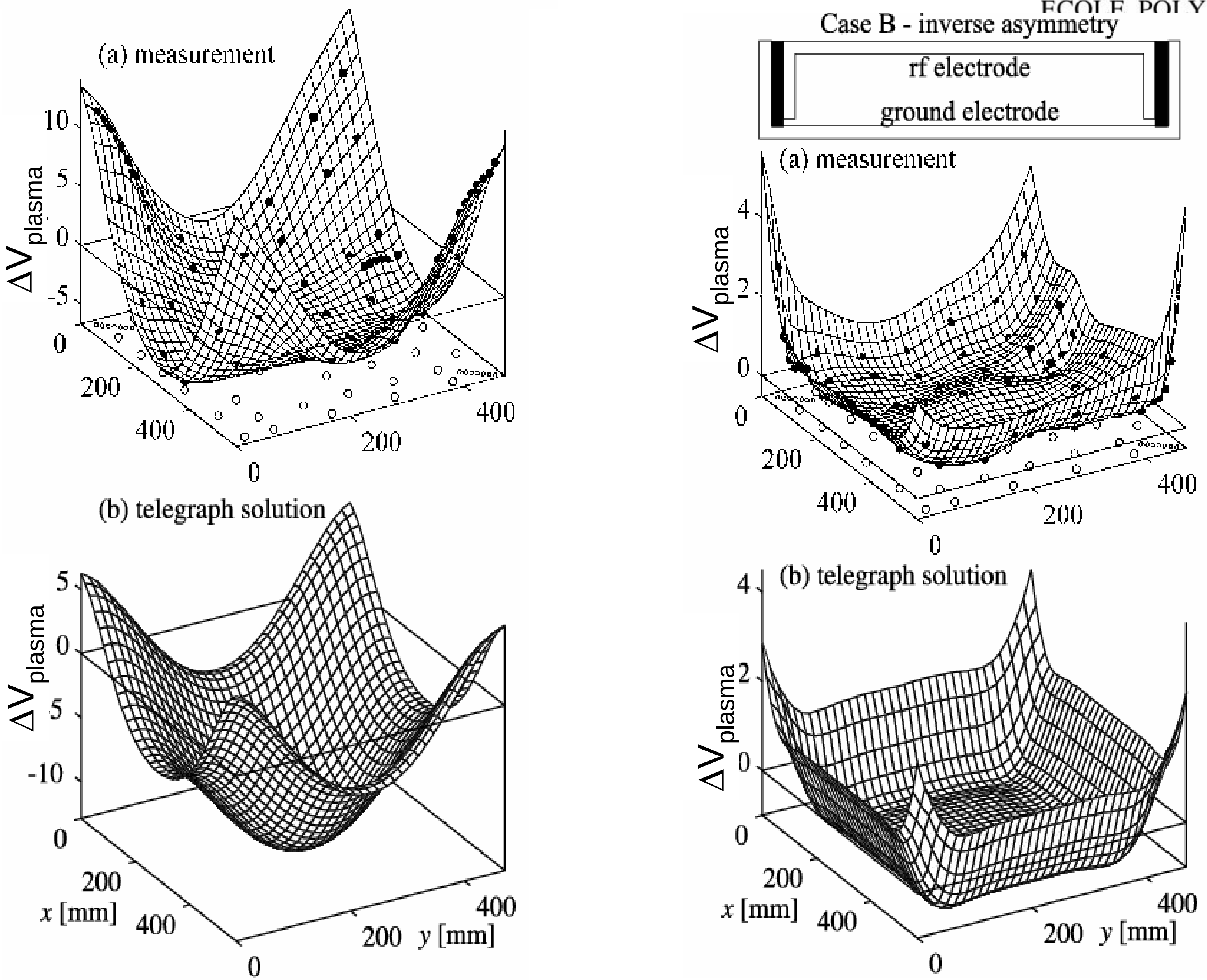


At mid-point, good correspondence of
- **1D analytic solution**
- **2D numerical solution**
- **experimental measurements**

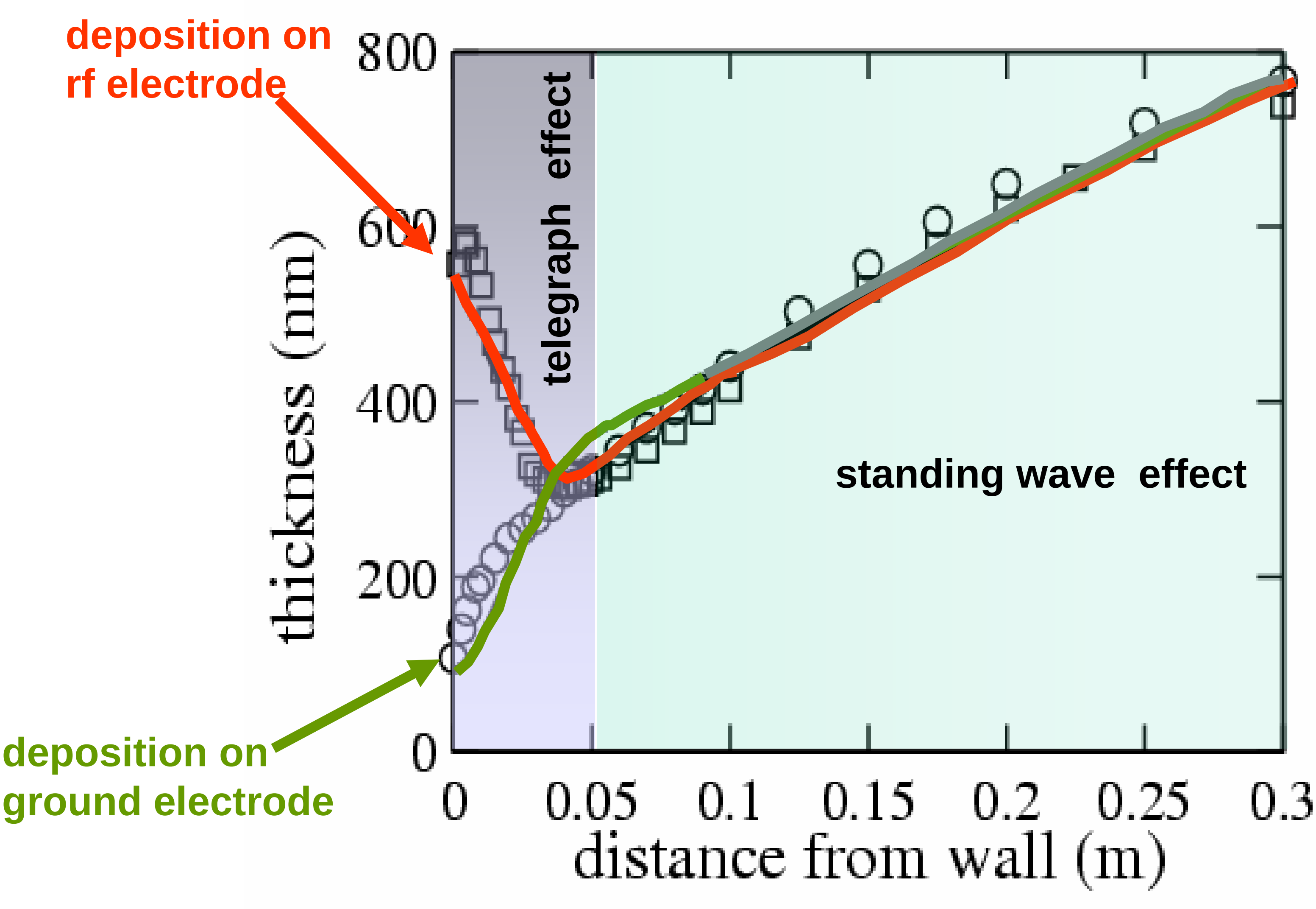


2D calculation of the telegraph effect in rectangular reactors

JOURNAL OF APPLIED PHYSICS 97, 123308 (2005)



2D calculation of film thickness profiles



2D Fluid equations for plasma

ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

electron continuity: $\dfrac{\partial n_{\mathrm{e}}}{\partial t}+\nabla\cdot\underline{\Gamma}_{\mathrm{e}}=k_{\mathrm{ion}}n_{\mathrm{e}}N;\quad \underline{\Gamma}_{\mathrm{e}}=-\mu_{\mathrm{e}}n_{\mathrm{e}}\underline{E}-D_{\mathrm{e}}\nabla n_{\mathrm{e}}$

ion continuity: $\dfrac{\partial n_{\mathrm{i}}}{\partial t}+\nabla\cdot\underline{\Gamma}_{\mathrm{i}}=k_{\mathrm{ion}}n_{\mathrm{e}}N;\quad \underline{\Gamma}_{\mathrm{i}}=\mu_{\mathrm{i}}n_{\mathrm{i}}\underline{E}-D_{\mathrm{i}}\nabla n_{\mathrm{i}}$

electron energy continuity; $(n_{\mathrm{e}}\varepsilon)$ is the energy density in $\mathrm{eV}\cdot\mathrm{m}^{-3}$:

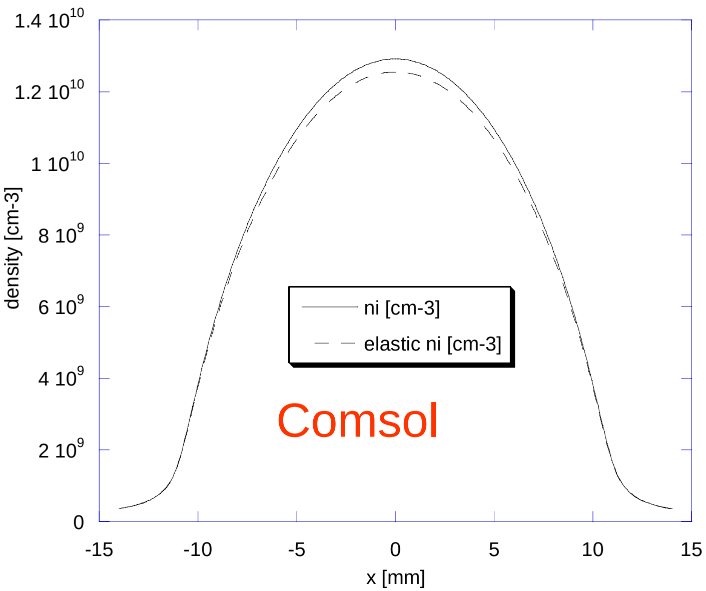
$$\frac{\partial(n_{\mathrm{e}}\varepsilon)}{\partial t}+\nabla\cdot\underline{\Gamma}_{\mathrm{w}}=-\underline{\Gamma}_{\mathrm{e}}\cdot\underline{E}-K_{\mathrm{loss}}n_{\mathrm{e}}N;\quad \underline{\Gamma}_{\mathrm{w}}=-\frac{5}{3}\mu_{\mathrm{e}}(n_{\mathrm{e}}\varepsilon)\underline{E}-\frac{5}{3}D_{\mathrm{e}}\nabla(n_{\mathrm{e}}\varepsilon);$$

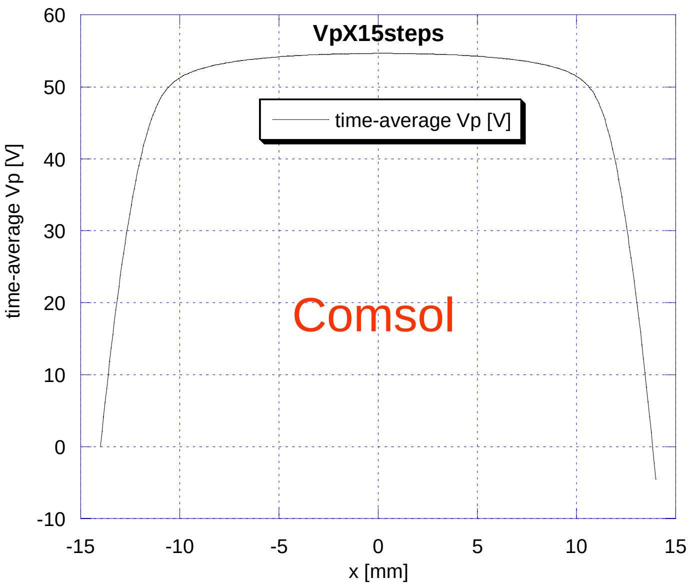
$$-\underline{\Gamma}_{\mathrm{e}}\cdot\underline{E}=\mu_{\mathrm{e}}n_{\mathrm{e}}\left(E_x^2+E_y^2\right)+D_{\mathrm{e}}\left(\frac{\partial n_{\mathrm{e}}}{\partial x}E_x+\frac{\partial n_{\mathrm{e}}}{\partial y}E_y\right).$$

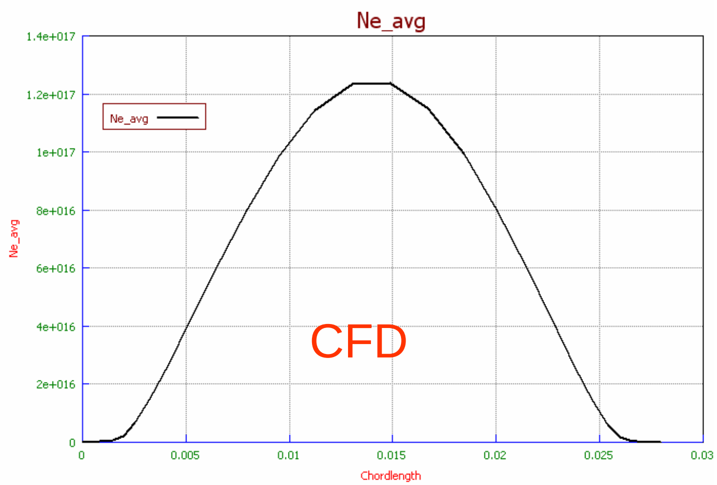
Poisson's equation: $\nabla^2 V=-\dfrac{\mathrm{e}}{\varepsilon_0}(n_{\mathrm{i}}-n_{\mathrm{e}});\quad \underline{E}=-\nabla V$

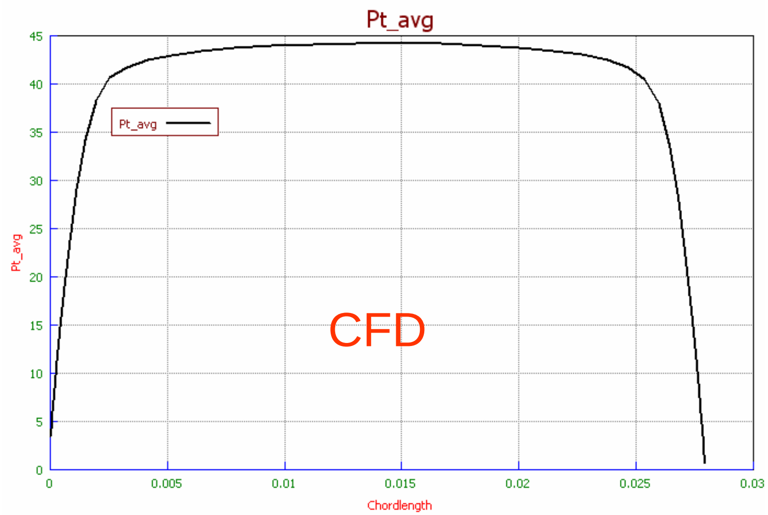
Time-averaged density profiles

Time-averaged plasma potential profiles









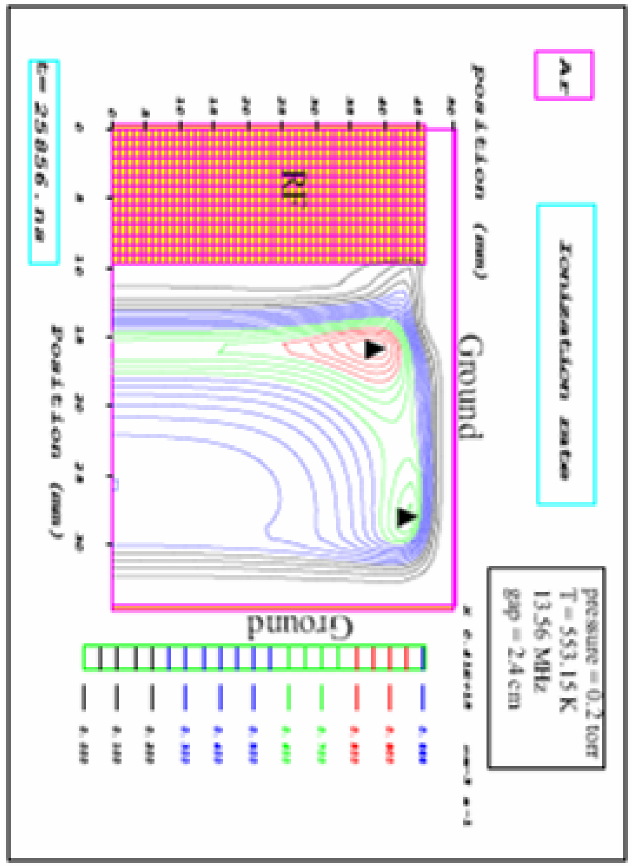
4) NUMERICAL SIMULATION (eg Siglo-RF; and COMSOL Multiphysics finite elements)

- Siglo 2D plasma simulation: edge and telegraph

- CFD showerhead uniformity, compare 0D plasma chemistry

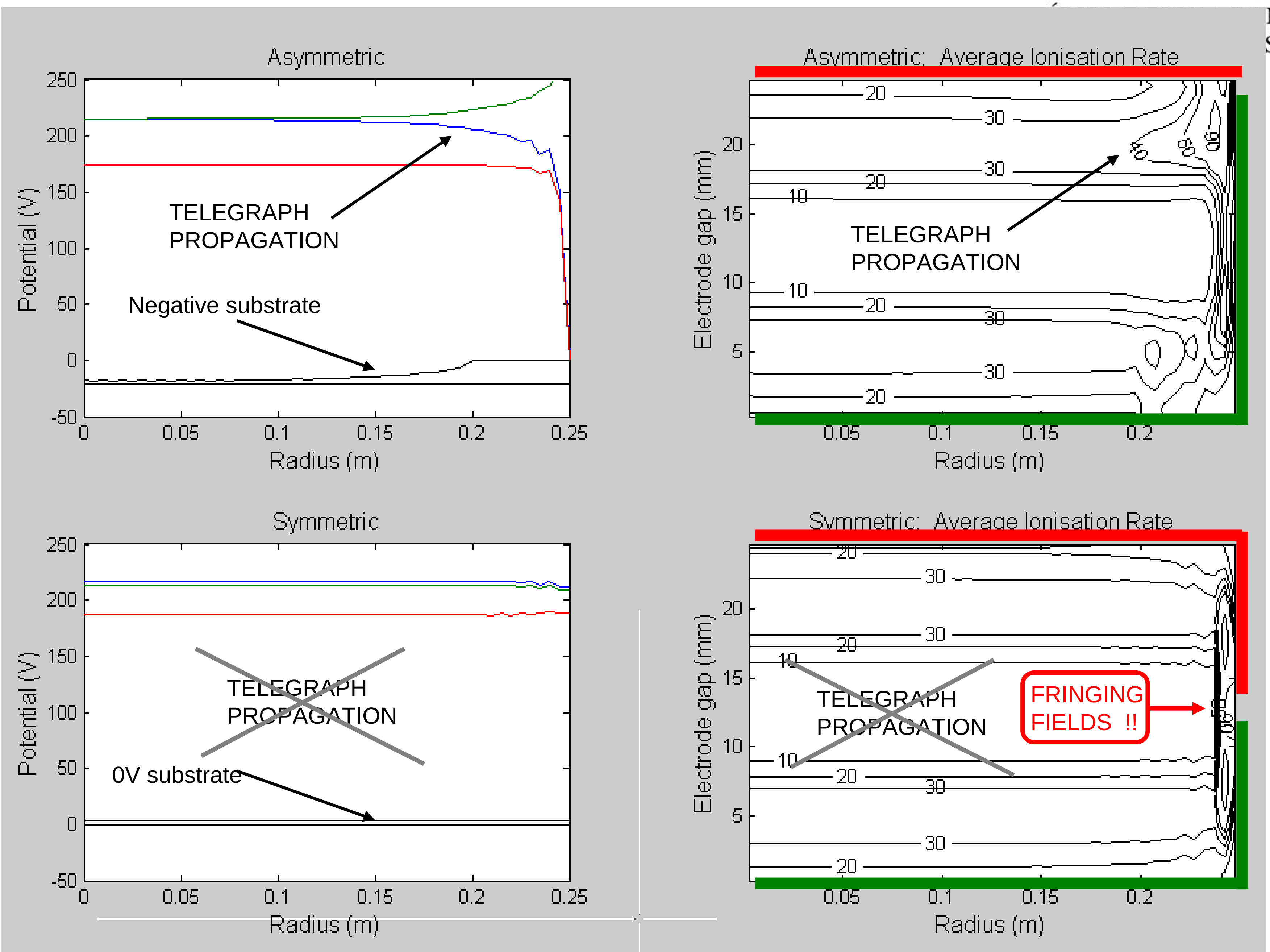
- Comsol gas flow, edge speed

Siglo2D simulation of plasma ionization rate for a standard edge geometry.



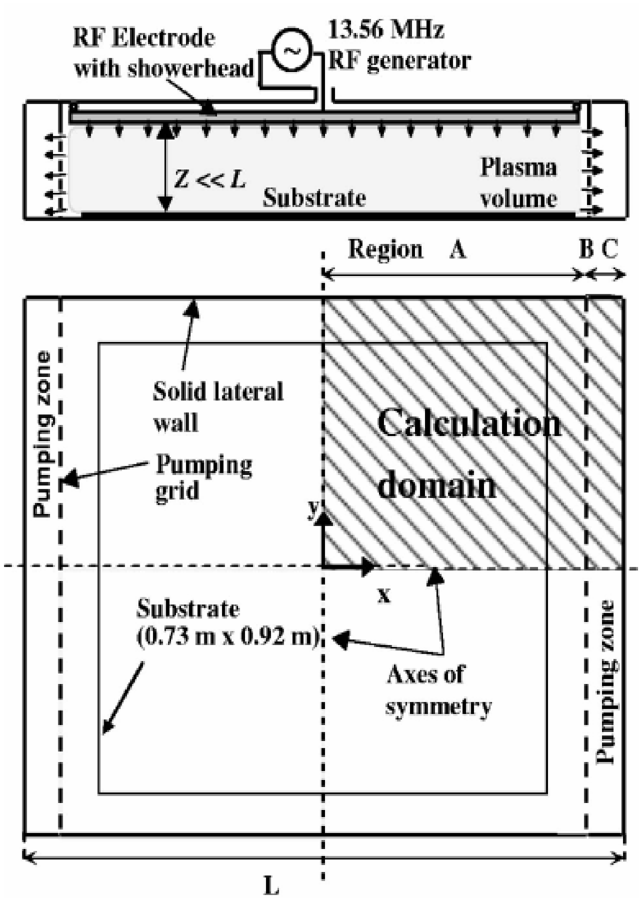
Plasma simulation : SIGLO-2D

J. Appl. Phys. **96**, 5429 (2004)



CFD-ACE

R. Sobbia *et al, J.Vac.Sci.Technol.* **A23**, 927 (2005)



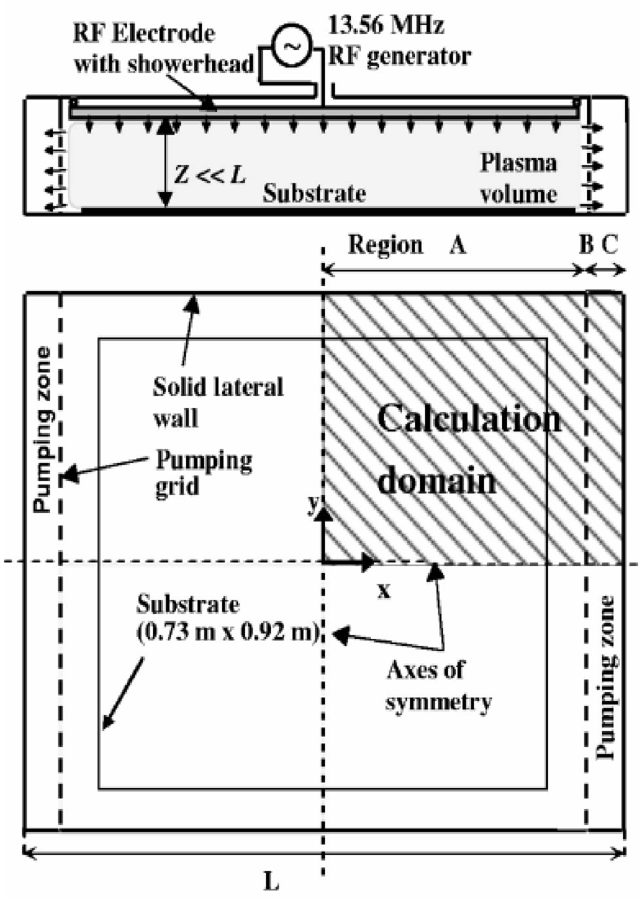
3D, silicon nitride deposition.

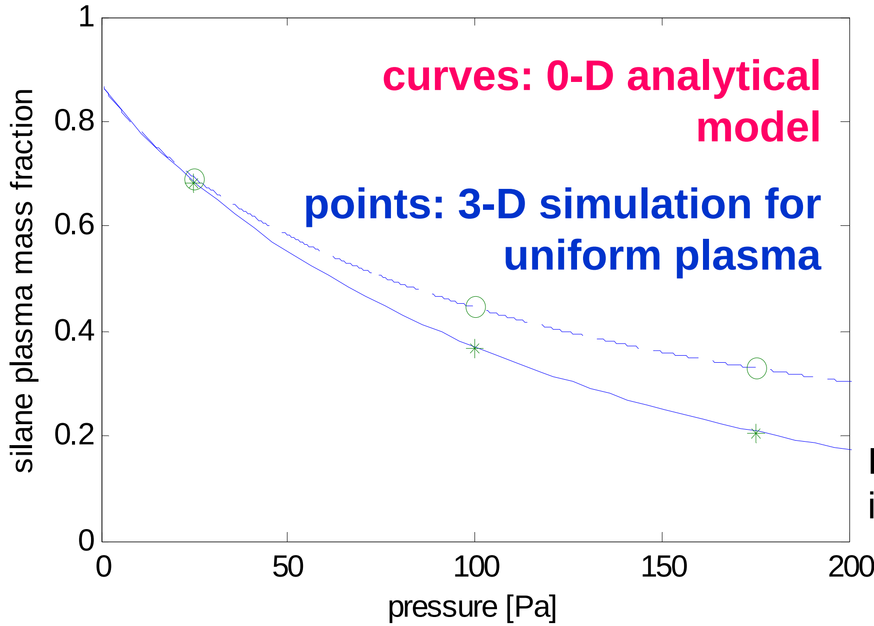
Gas injection, standing wave and telegraph effect are calculated separately.

Number	Reaction	Rate constant (s^{-1} m^3)
	Electron impact dissociations	
(R1)	$e^- + NH_3 \rightarrow NH_2 + H + e^-$	9.0×10^{-16}
(R2)	$e^- + SiH_4 \rightarrow SiH_2 + 2H + e^-$	1.9×10^{-16}
(R3)	$e^- + SiH_4 \rightarrow SiH_3 + H + e^-$	1.5×10^{-16}
(R4)	$e^- + Si_2H_6 \rightarrow SiH_4 + SiH_2 + e^-$	4.7×10^{-16}
	Reactions with silane	
(R5)	$SiH_4 + NH_2 \rightarrow SiH_3 + NH_3 + H$	4.0×10^{-18}
(R6)	$SiH_4 + NH_2 \rightarrow SiH_2NH_2 + H_2$	1.0×10^{-17}
(R7)	$SiH_4 + SiH_2 \rightarrow Si_2H_6$	1.0×10^{-17}
	Reactions between radical species	
(R8)	$NH_2 + H_2 \rightarrow NH_3 + H$	1.0×10^{-18}
(R9)	$SiH_2 + H_2 \rightarrow SiH_4$	2.0×10^{-19}
(R10)	$SiH_2 + NH_2 \rightarrow SiH_2NH_2$	7.8×10^{-17}
(R11)	$SiH_3 + SiH_3 \rightarrow SiH_4 + SiH_2$	1.5×10^{-16}
(R12)	$SiH_3 + NH_2 \rightarrow SiH_2 + NH_3$	2.1×10^{-17}
(R13)	$SiH_2NH_2 + NH_2 \rightarrow Si(NH_2)_2 + H_2$	9.8×10^{-17}
(R14)	$Si(NH_2)_2 + NH_2 \rightarrow Si(NH_2)_3$	1.0×10^{-16}
	Reactions with disilane	
(R15)	$Si_2H_6 + NH_2 \rightarrow Si_2H_5 + NH_3$	1.7×10^{-17}
(R16)	$Si_2H_5 + NH_2 \rightarrow SiH_4 + SiHNH_2$	1.0×10^{-16}
(R17)	$Si_2H_6 + H \rightarrow Si_2H_5 + H_2$	6.5×10^{-18}
	Surface (S) mechanisms	Sticking coefficient
(S1)	$H + H + S \rightarrow H_2$	1
(S2)	$NH_2 + S \rightarrow N(S) + H_2$	0.02
(S3)	$SiH_2 + S \rightarrow Si(S) + H_2$	0.8
(S4)	$SiH_2 + NH_2 + S \rightarrow Si-N(S) + 2H_2$	0.005
(S5)	$SiH_3 + S \rightarrow Si(S) + H_2 + H$	0.05
(S6)	$Si_2H_5 + S \rightarrow Si(S) + 2H_2 + H$	0.05
(S7)	$Si(NH_2)_2 + S \rightarrow N-Si-N(S) + 2H_2$	0.02
(S8)	$Si(NH_2)_3 + S \rightarrow N-Si-N(S) + NH_3 + H_2 + H$	0.003

CFD-ACE

R. Sobbia *et al, J.Vac.Sci.Technol.* **A23**, 927 (2005)





H abstraction included

Navier-Stokes $\nabla \cdot (\rho \mathbf{v}\mathbf{v}) = -\nabla p + \nabla \cdot (\mu \nabla \mathbf{v}),$

Species continuity $\nabla \cdot (\rho \mathbf{v} Y_i) = -\nabla \cdot \mathbf{J}_i + R_i + S_i,$

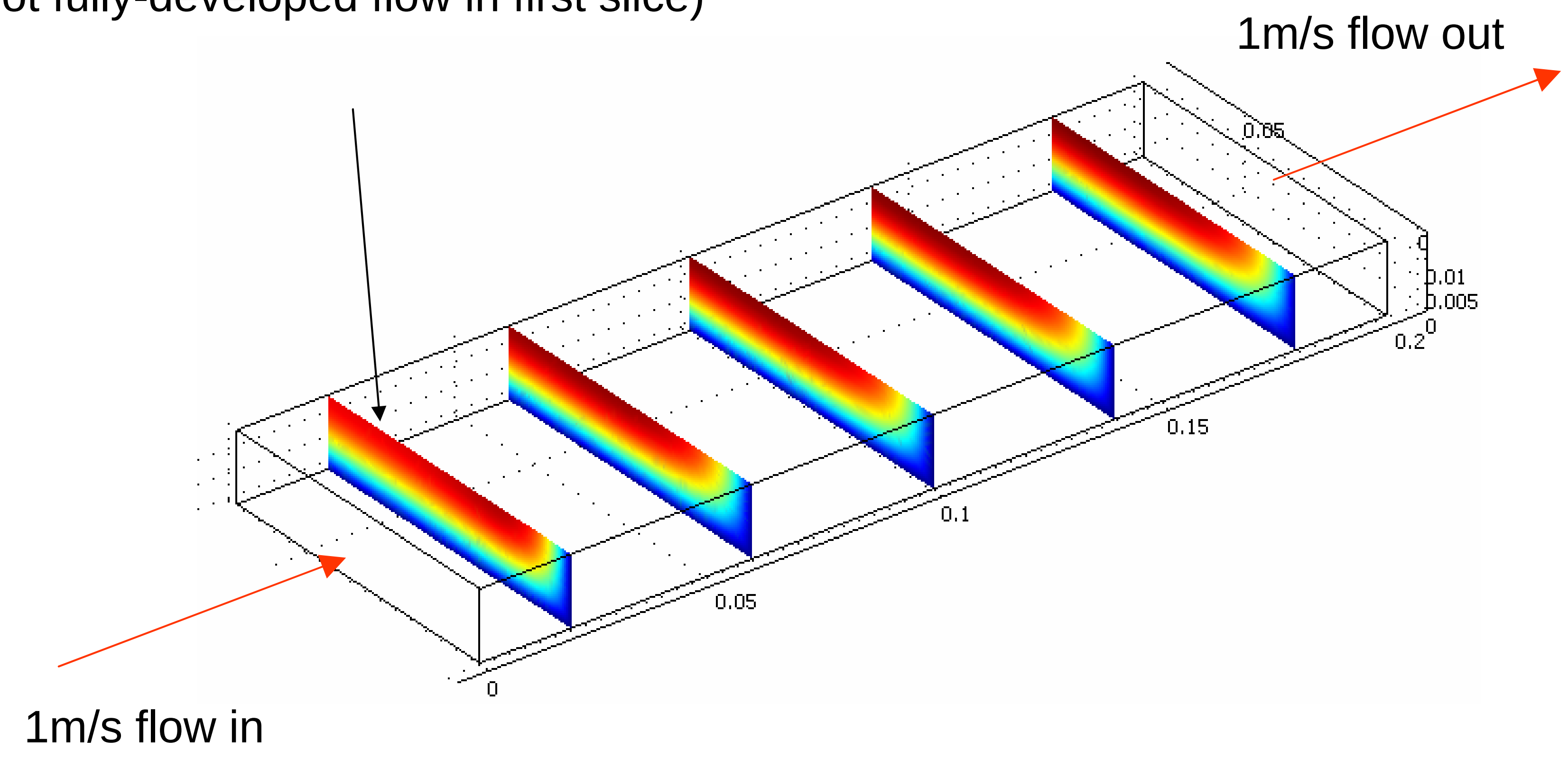
Diffusive mass flux $\mathbf{J}_i = \mathbf{J}_i^C = -\rho D_i^{\mathrm{eff}} \nabla Y_i + M Y_i D_i^{\mathrm{eff}} \sum_{j=1, j\neq i}^{N} \frac{\mathbf{J}_j^C}{M_j D_{ij}}$

Comsol for Navier-Stokes numerical simulations:

for example, channel flow

Half-height, edge region

(not fully-developed flow in first slice)

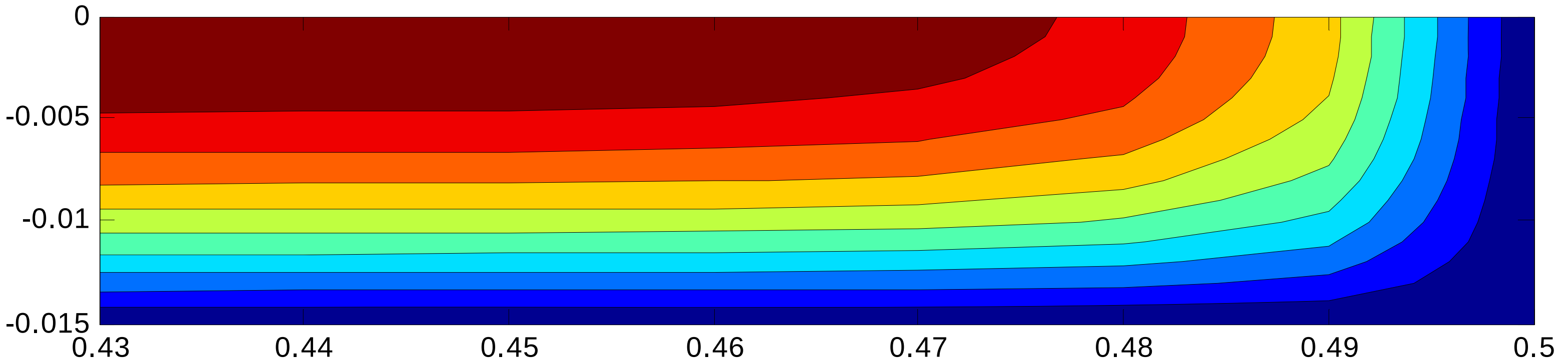


Compare analytical expression (using Matlab)
with numerical simulation above (Comsol, Navier-Stokes)

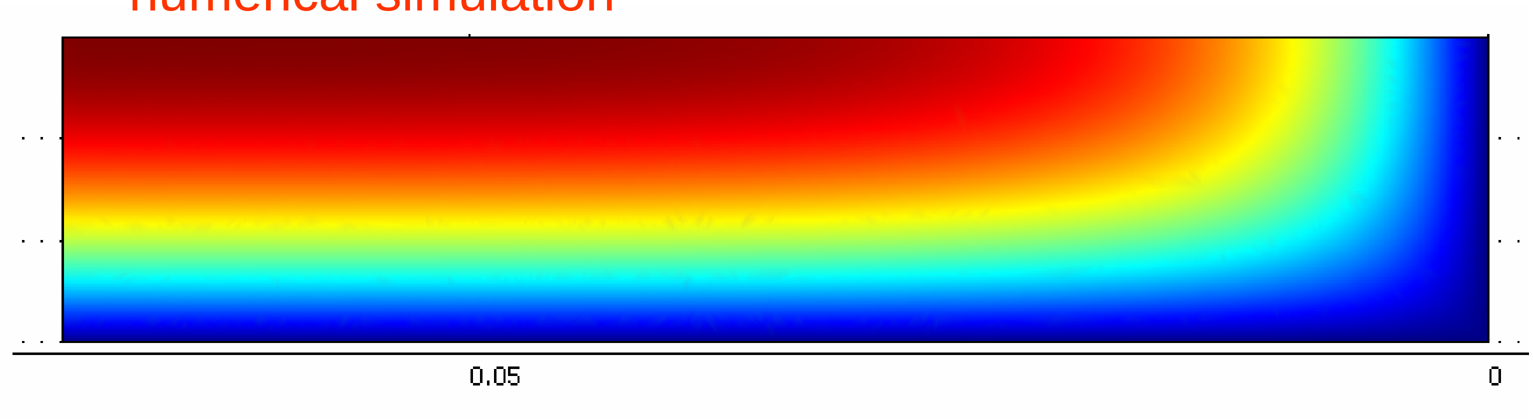
$$u(y,z)=\frac{16a^2}{\mu\pi^3}\left(-\frac{dp}{dx}\right)\sum_{i=1,3,5\ldots}^{\infty}\frac{(-1)^{(i-1)/2}}{i^3}\left[1-\frac{\cosh(i\pi z/2a)}{\cosh(i\pi b/2a)}\right]\cos\left(\frac{i\pi y}{2a}\right)$$

in F. M White "Viscous Flow" McGraw-Hill, NY

analytic expression



numerical simulation



CONCLUSION: Analytic solutions still have a wide application, even in a numerical world!